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Revision 1

Characterization Of Tank WM-189 Sodium-Bearing Waste At The Idaho Nuclear Technology And Engineering Center

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Idaho National Engineering and Environmental Laboratory
Bechtel BWXT Idaho, LLC

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SUMMARY

Idaho Nuclear Technology and Engineering Center 300,000-gallon vessel WM-189 was filled in late 2001 with concentrated sodium bearing waste (SBW). Three airlifted liquid samples and a steam jetted slurry sample were obtained for quantitative analysis and characterization of WM-189 liquid phase SBW and tank heel sludge. Estimates were provided for most of the reported data values, based on the greater of (a) analytical uncertainty, and (b) variation of analytical results between nominally similar samples.

A consistency check on the data was performed by comparing the total mass of dissolved solids in the liquid, as measured gravimetrically from a dried sample, with the corresponding value obtained by summing the masses of cations and anions in the liquid, based on the reported analytical data. After reasonable adjustments to the nitrate and oxygen concentrations, satisfactory consistency between the two results was obtained. A similar consistency check was performed on the reported compositional data for sludge solids from the steam jetted sample.

In addition to the compositional data, various other analyses were performed: particle size distribution was measured for the sludge solids, sludge settling tests were performed, and viscosity measurements were made.

WM-189 characterization results were compared with those for WM-180, and other Tank Farm Facility tank characterization data.

A 2-liter batch of WM-189 simulant was prepared and a clear, stable solution was obtained, based on a general procedure for mixing SBW simulant that was develop by Dr. Jerry Christian. This WM-189 SBW simulant is considered suitable for laboratory testing for process development.

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Thanks to Dr. Jerry Christian, for his tutelage and insight. Special thanks to Bob Kirkham for his invaluable advise on the data modeling. Finally, to Arlin Olson — his standards are the benchmark of excellence. To this end, we hope that the information presented here is useful, and others can build upon it.

CONTENTS

FIGURES

TABLES

ACRONYMS

ACMM	Analytical Chemistry Methods Manual
ALD	Analytical Laboratories Department
DOE	Department of Energy
EDMS	Electronic Document Management System
ERDL	Environmental Research and Development Laboratory
EPA	Environmental Protection Agency
HLLWE	High Level Liquid Waste Evaporator
HLW	High Level Waste
INEEL	Idaho National Engineering and Environmental Laboratory
INTEC	Idaho National Technology and Engineering Center
LDUA	Light Duty Utility Arm
NRC	Nuclear Regulatory Commission
NWCF	New Waste Calcining Facility
PSD	particle size distribution
RAL	Remote Analytical Laboratory
RCRA	Resource Conservation and Recovery Act
SAP	Sampling and Analysis Plan
SBW	Sodium Bearing Waste
SEM	Scanning Electron Microscope
SVOA	Semi-Volatile Organic Analysis
TEM	Transmission Electron Microscope
TDS	Total Dissolved Solids
TFF	Tank Farm Facility
UDS	Undissolved Solids
US-DOE	U.S. Department of Energy
VOA	Volatile Organic Analysis
WIR	Waste Incidental to Reprocessing

Characterization of Tank WM-189 Sodium-Bearing Waste at the Idaho Nuclear Technology and Engineering Center

1. BACKGROUND AND INTRODUCTION

Reprocessing of Spent Nuclear Fuel (SNF) began at the Idaho Chemical Processing Plant, ICPP (now the Idaho Nuclear Technology and Engineering Center, INTEC) in 1953. This reprocessing produced mixed[a] liquid waste, which was stored in the Tank Farm Facility (TFF). Since 1963, most of this liquid waste has been removed from the TFF and solidified using a process called calcination.

A variety of SNF types were processed at INTEC. Two types of liquid waste have been stored - high level waste (HLW) and sodium bearing waste (SBW). The HLW was generated as a direct result of reprocessing SNF. The composition of the HLW was dependent on the fuel type being processed, with aluminum, zirconium, and Fluorinel producing the greatest volumes of waste. The SBW was generated from incidental activities, such as reprocessing solvent cleanup and decontamination, associated with operation of INTEC. The name "Sodium Bearing Waste" and its distinction as a separate liquid waste form is in recognition of the waste's high concentration of sodium ion which is problematic to calcination (primarily due to bed agglomeration). The sodium resulted from processing and decontamination activities that made extensive use of sodium-based chemicals such as sodium hydroxide and sodium carbonate.

The TFF consists of eleven nominal 300,000-gallon stainless steel tanks enclosed in concrete vaults and ancillary equipment. The tanks are numbered WM-180 through WM-190. WM-190 has been maintained as a spare. In late 2000 a waste management plan (the 2070 Plan, Ref. 1) was developed to document the plans for liquid waste stored in the Tank Farm, liquid wastes that would continue to be generated, and calcine stored in Bin Sets. Among other items, the 2070 Plan:

- Describes the history of waste generation at INTEC
- Discusses the equipment and processes which have treated and will continue to treat INTEC wastes
- Discusses and provides estimates of new waste generation volumes
- Discusses the computer model used for waste treatment planning
- Discusses the schedule for emptying and closing Tank Farm tanks

Several original assumptions have changed since this plan was issued. However, the INEEL HLW Program has been making progress towards consolidating all of the tank liquids and heels into four tanks; WM-180, -187, -188, and -189. It is intended to collect wash solutions and heels from TFF closure activities in WM-187. WM-180 has been filled and a characterization effort has been performed for that tank (Ref. 2), and WM-188 is being filled. WM-189 was filled early in Fiscal Year 02.

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a. Mixed is a regulatory term for waste that contains both radioactive and hazardous constituents. The hazardous constituents are defined in the Resource Conservation and Recovery Act (RCRA). Both listed and characteristic components, as defined by RCRA, are contained in the INTEC waste.

It is important to have liquid and heel solids characterization data from the TFF in order to perform process design and development activities for the SBW treatment and disposal alternatives, and to support selection of the preferred alternative. The data are utilized to develop non-radioactive simulants to support the process development efforts. It is also important to have this data to support preliminary permitting activities.

The scope of the activities reported here include the sampling, analytical analyses, and analysis of the data for Tank WM-189.

2. PURPOSE AND SCOPE

2.1 Data Need

The Department of Energy (DOE) and the Idaho National Engineering and Environmental Laboratory (INEEL) must make decisions regarding the management of wastes stored in the TFF that will meet the milestones and intent set forth in the Settlement Agreement, Consent Orders, and the Site Treatment Plan (STP). The decision to be supported by the sampling/analysis activity described here is to choose a preferred treatment option for the liquid wastes described in Section 1. That decision will be based on comparisons of performance and costs of different process alternatives. Process performance and implementation costs will likely be driven by the waste composition. Hence, the validity of the choice of a treatment option will depend on the quality of the waste characterization data used for the above comparisons. Likewise, data quality is vitally important for permitting activities.

Not only may the treatment and disposal requirements be dictated by contaminants in the waste, but also a permitting strategy may be driven by the quality of the data itself. Decisions in both arenas will be driven by confidence in the accuracy of the data. Thus, the validity of any decisions made with the waste characterization data as input will depend on the quality of that data.

2.2 Scope of Sampling/Analysis

The DOE, recognizing the importance of characterization to their management effort, incentivized this sampling/analysis activity to the INEEL operating contractor, Bechtel BWXT Idaho, LLC (BBWI). A Performance Based Incentive (PBI) was established under PBI-5 Empty and Close HLW Tanks. It is listed as *PBI-5 Expectation 1.2: Characterize the liquid contents of WM-188 and WM-189 to support SBW treatment*. The milestone is "During FY02, characterize the liquid contents of tank WM-189," due on September 30, 2002. Completion is defined as "Submit the waste characterization and evaluation report of Tank WM-189, with a comparison of results to WM-180 waste characterization data." The present report is intended to fulfill the expectations of that PBI.

The overall scope of this characterization effort was to sample Tank WM-189 and obtain chemical and radiochemical composition data of known quality for liquid and sludge. More specifically, samples were to be collected that are representative of the liquids and sludge in the tanks. The compositions of these samples were then to be determined and the results reported, together with credible estimates of their uncertainties. Prior to sampling WM-189, a *sampling and analysis plan* (SAP) was generated, reviewed, approved, and issued—"SBW Sampling and Analysis Plan," PLN-1027 (Ref. 3). This plan provides for 'RCRA protocol' sample preparation and analyses (as practicably achievable) of the SBW at the INTEC. In brief the plan provided the following provisions:

- Samples were to be obtained from Tank WM-189 at the INTEC
- Samples were to be collected, prepared, and analyzed according to RCRA protocol (subject to limitations due to the radioactive environment)
- A list of target analytes was identified together with specific methods to be used in characterization activities
- Reporting requirements were specified.

Specific objectives from this activity are as follows:

1. Determine from sampling and analysis representative nominal concentrations of the target analytes (radioactive and non-radioactive) from Ref. 3 in liquid waste from WM-189 at the INTEC TFF.

2. Determine from sampling and analysis representative nominal concentrations of the target analytes from Ref. 3 in sludge from WM-189 at in the INTEC TFF.

3. Provide quantitative measures of the quality of the data provided in items 1 and 2.

4. Compare the characterization data for WM-189 with corresponding data for WM-180.

3. SAMPLING, ANALYSIS, AND RESULTS

3.1 Sampling

Sampling of WM-189 was unique because WM-189 has an airlift transfer system that was used for some of the samples. It also has a steam jet transfer system (Other tank farm vessels have *only* a steam jet system). WM-189 sampling included three airlift samples (designated as "Sample 1, "Sample 2", and "Sample 3") and a single steam-jetted bottom sample (designated the "Bottom Sample"). The airlift system differs from the steam jet system in that (a) the principal suction point in the tank is ~10 ft above the tank bottom (vs. ~2 inches from the bottom for the steam jet), and (b) there is no water dilution with the airlift system. Table 3-1 provides a summary of the samples that were collected, their origins, types, and the analyses performed.

WM-189 sampling activities commenced on March 8, 2002. Three separate ~300 gallon flushes of WM-189 solution were transferred through the NWCF NCC-101 sampling vessel equipment utilizing the WM-189 airlift. This ensured that extraneous solutions were flushed from the sampling transfer lines and equipment. It also ensured that any remaining/residual solution was essentially the same as the WM-189 solution in the forthcoming sampling events. Three separate 1,000-gallon batches were airlifted into the NCC-101 sampling vessel. From each of these batches, approximately one liter of solution was drawn while NCC-101 was under a fully agitated condition provided by an air sparge. Each one-liter volume constituted a single sample that was then transported to the INTEC Remote Analytical Laboratory (RAL) where it was prepared for analyses. The batch remaining in NCC-101 was then flushed back to the tank farm (NOT WM-189) so that the next batch of WM-189 tank solution could be transferred in for sampling. Once the airlift samples were secured, the Bottom Sample was taken utilizing the steam jet. As anticipated from the sampling location, the steam jet sample contained some solids (the airlift samples did not). Additional details of these sampling activities are given in Appendix A. Due to a broken manipulator at the RAL, the Bottom Sample was not received there until April 16, 2002. All airlift samples were received at the RAL within 24 hrs of being drawn.

From visual observation it was assumed that there were negligible solids present in Samples 1, 2, and 3; hence, no solids separation was performed on these samples. The Bottoms Sample, however, contained a significant fraction of sludge, which was partially separated from the liquid as described below in Section 3.2.2.

Table 3-1. WM-189 samples collected and analytical procedures used to characterize them.

Sample Identifier	Sampling Location	Sample Type	Analyses Performed (see Table 3-2)
Sample 1	Airlift	Liquid only	7981, 7004, 8060, 9260, 9270, 7012, 2111, 2809, 2900, 8100
Sample 2	Airlift	Liquid only	7981, 7004, 8060, 9260, 9270, 7012, 2111, 2809, 2900, 8100
Sample 3	Airlift	Liquid only	3011, 3000, 3381, 3993, 3431, 3539, 3209, 3204, 3202, 3201, 3203
Bottom Sample	Steam jet	Slurry	8968, 2007, 2702, 7981, 8060, 9260, 9270, 7012, 2111, 2809, 2900, 8100

3.2 Analysis

The INEEL Analytical Laboratories Department (ALD) analyzed the WM-189 samples utilizing the ALD Analytical Chemistry Methods Manual (ACMM) procedures. Wherever possible, analyses were performed with EPA SW-846-equivalent (Ref. 4) ACMM's. Descriptions for the ACMM procedures can be found on Web at the ALD homepage (http://dune.inel.gov/). A cross-reference between the SW-846 protocol methods and the ACMM methods is detailed in ALD's Quality Assurance Project Plan for the Analysis of Environmental Samples, PLN-407 (Ref. 5). Final analytical data (inorganic, organic, and radiological) was issued in Tier 2 reports per PLN-1027. The HLW Sample Coordinator provides a record copy of the Tier 2 reports to the HLW & ERDL Central Files Record Storage Coordinator for retention.

3.2.1 Liquid Samples

Sample 1 and Sample 2 were analyzed by RCRA protocol for non-radioactive liquid phase analytes listed in Ref. 3. Sample 3 was analyzed for liquid phase radionuclides using INTEC process sample protocol. Liquid from the Bottom Sample was analyzed for both non-radioactive analytes (again per RCRA protocol) and radionuclides. A complete list of the analysis procedures utilized for the WM-189 samples is presented in Table 3-2.

3.2.2 Slurry Sample

There is no EPA-established protocol for preparation of a slurry prior to a fusion; nor does the Method 8108 description provide any specific procedure for preparation of a slurry. For these reasons the following method was devised to extract and prepare both a liquid and a sludge sample from the WM-189 Bottom Sample slurry.

Approximately 165 mL of 'as received' Bottom Sample slurry was set aside for analysis. The sample slurry was comprised of a supernatant liquid layer and a settled sludge layer. The sludge layer was comprised of undissolved solid particles and interstitial liquid. After a 24-hr settling time the supernatant liquid above the sludge layer was carefully taken off and a sample was separated for analysis. Analyses were performed on this liquid sample as discussed in Section 3.2.1. A 15 mL aliquot of sludge was extracted from the sludge layer and was utilized for chemical/radiochemistry analyses as described in Table 3-1. The remaining sludge (~7 mL) was retained for measurement of the particle size distribution (psd) of the sludge solids.

Interstitial liquid was not separated from the gravity settled sludge sample. The 15 mL sludge aliquot (comprised of the UDS plus interstitial liquid, including dissolved solids) was dried per ACMM-7004 and fused per ACMM-8108. The dried, fused solids were then dissolved in nitric acid or water and the same analytical methods used for the liquid phase analyses were applied to measure concentrations of sludge constituents. The chemical and radiochemistry analyses on this dried sludge material were done in duplicate and the results termed 'Fusion1' and 'Fusion2'.

3.3 Results

3.3.1 Liquid Phase Analyses

Liquid phase analytical results on the WM-189 samples are presented in this section. Samples 1 and 2 and the Bottom Sample were used to obtain all non-radioactive analytical results. Radiochemical analyses for the liquid phase were performed using Sample 3 and the Bottom Sample.

Table 3-2. ACMM method number and analyses.

ACMM Method Number	Analysis/Analyte
7981	Specific Gravity (SpGr)
7004	Total Dissolved Solids (TS or TDS)
8968	Particle Size Distribution (psd)
2007	Scanning Electron Microscope – Energy Dispersive Spectrometry (SEM – EDS)
2702	X-Ray Diffraction (XRD)
8060	Total Organic Carbon (TOC, TIC)
9260	Total VOA (Volatile Organic Analysis)
9270	Total SVOA (Semi-Volatile Organic Analysis)
7012	Acid (H^+)
2111	Cesium (Cs)
2809	Mercury (Hg)
2900	All Other Metals
8100	Anions (F, Cl, NO_3, SO_4, PO_4)
8108	Fusions
3011	Tritium
3000	Carbon-14, Nickel-59, Nickel-63, Plutonium-241
3381	Total Strontium
3993	Europium-154, Cesium-134, Cesium-137, Cobalt 60, Niobium-94, Zirconium-95
3431	Technetium-99
3539	Iodine-129
3209	Uranium-234, -235, -236, -238
3204	Neptunium-237
3202	Plutonium-238, -239
3201	Americium-241
3203	Curium-242, -244

Non-radioactive data for Samples 1 and 2 and the Bottom Sample liquid are presented in Table 3-3. This data was obtained by importing raw analytical data directly from the ALD's computer system where it is reported as mass of analyte per unit volume of liquid. The ALD data is reported here. In the case of the Bottom Sample liquid, the mass concentrations were adjusted to account for a dilution of 2.8% from

the steam transfer system.[b] Table 3-3 lists the nominal measured concentrations for all three samples in columns 2-4. Column 5 gives the average of the three sample values and is the recommended nominal value for the tank. An estimate of the uncertainty (as a percentage) that should be attached to the nominal value is presented in column 6. The bases for the uncertainty values are provided in the footnotes to the table; the largest uncertainty value is presented. VOA (TOTAL) and SVOA (TOTAL) values were determined from the respective Tier 2 reports. These values were the sum of the compounds that had 'hits'; these organic data are presented in Appendix B. [Note: In addition to the data in Table 3-3, Scanning Electron Microscope (SEM) *energy dispersive spectrometry* (EDS) (ACCM-2007) was used to obtain some elemental analysis on the dried total dissolved solids from Sample 3. This data is considered to be qualitative only but is provided in Appendix B.]

Liquid phase radionuclide concentrations for Sample 3 and the Bottom Sample are reported in Table 3-4. Similar reporting conventions to those in Table 3-3 have been used.

Table 3-3. WM-189 non-radioactive species concentrations in liquid from Sample 1, Sample 2, and Bottom Sample; Units are mg/L (SpGr is @ 25/4).

Constituent or Property	Sample1 Results	Sample2 Results	Bottom Sample Results	Recommended Value	Value Uncertainty	
SPGR	1.33501	1.33315	1.36117	1.34311	1.2%	(2)
UDS (TSS)	NA	NA	NA	-	-	-
TIC	NA	NA	10.0	-	-	-
TOC	624	625	513	587	11%	(2)
VOA (TOTAL)	0.10	9.2E-02	0.30	0.16	73%	(2)
SVOA (TOTAL)	1.0	0.24	2.0	1.1	83%	(2)
Remote TS (AIR)	5.13E+05	4.98E+05	NA	5.06E+05	2%	(2)
Remote TS (OVEN)	2.91E+05	2.85E+05	NA	2.88E+05	1%	(2)
Acid	2.9E+03	2.9E+03	2.9E+03	2.9E+03	6%	(1)
Aluminum	1.95E+04	1.92E+04	1.94E+04	1.94E+04	10%	(3)
Antimony	1.14E+00	7.47E-01	8.83E-01	9.24E-01	22%	(2)
Arsenic	ND	ND	5.81E-01	IDL= 0.333	-	-
Barium	7.95E+00	7.41E+00	8.03E+00	7.80E+00	10%	(3)
Beryllium	1.82E-01	1.82E-01	1.87E-01	1.83E-01	10%	(3)
Boron	2.24E+02	2.21E+02	2.48E+02	2.31E+02	10%	(3)
Cadmium	4.49E+02	4.31E+02	4.50E+02	4.44E+02	10%	(3)
Calcium	2.95E+03	2.92E+03	2.99E+03	2.95E+03	10%	(3)
Cerium	4.53E+00	4.26E+00	6.12E+00	4.97E+00	20%	(2)

b. The 2.8% dilution factor is the arithmetic average of two independent estimates. The first (3.0%) was obtained by averaging the dilution factors for the ten most abundant species in the liquid. Estimates for the individual specie dilution factors were obtained by direct comparison of the Bottom Sample results with the averaged Sample 1 + Sample 2 results. The second estimate (2.7%) was based on the initial and final temperatures of the Bottom Sample (steam jetted) before and after transfer to NWCF. The latter estimate was provided by Mike Swenson.

Table 3-3. (continued).

Constituent or Property	Sample1 Results	Sample2 Results	Bottom Sample Results	Recommended Value	Value Uncertainty	
Cesium	3.65E+00	3.62E+00	3.50E+00	3.59E+00	10%	(3)
Chromium	3.01E+02	3.01E+02	2.85E+02	2.96E+02	10%	(3)
Cobalt	2.74E+00	2.77E+00	2.76E+00	2.76E+00	10%	(3)
Copper	6.27E+01	6.19E+01	5.88E+01	6.11E+01	10%	(3)
Gadolinium	2.17E+01	2.14E+01	2.09E+01	2.13E+01	10%	(3)
Hafnium	8.93E+01	8.59E+01	1.17E+02	9.74E+01	18%	(2)
Iron	1.51E+03	1.50E+03	1.53E+03	1.51E+03	10%	(3)
Lead	2.34E+02	2.46E+02	2.49E+02	2.43E+02	10%	(3)
Lithium	2.64E+00	2.56E+00	2.88E+00	2.69E+00	10%	(3)
Magnesium	5.42E+02	5.25E+02	5.60E+02	5.42E+02	10%	(3)
Manganese	1.08E+03	1.06E+03	1.10E+03	1.08E+03	10%	(3)
Mercury	1.18E+03	1.28E+03	1.49E+03	1.32E+03	20%	(3)
Molybdenum	2.66E+01	2.66E+01	2.82E+01	2.71E+01	10%	(3)
Nickel	1.38E+02	1.35E+02	1.39E+02	1.37E+02	10%	(3)
Niobium	ND	ND	ND	IDL= 23.1	-	-
Palladium	ND	ND	5.30E-01	IDL= 0.384	-	-
Phosphorus	6.64E+01	6.71E+01	6.02E+01	6.46E+01	10%	(3)
Potassium	8.59E+03	8.76E+03	9.30E+03	8.88E+03	10%	(3)
Ruthenium	1.73E+01	1.66E+01	1.88E+01	1.76E+01	10%	(3)
Selenium	8.28E-01	ND	ND	IDL= 0.364	-	-
Silicon	1.04E+01	9.44E+00	6.29E+00	8.69E+00	25%	(2)
Silver	ND	ND	2.60E-01	IDL= 0.202	-	-
Sodium	4.78E+04	4.79E+04	4.62E+04	4.73E+04	10%	(3)
Strontium	1.25E+01	1.14E+01	1.37E+01	1.25E+01	10%	(3)
Sulfur	2.74E+03	2.69E+03	2.90E+03	2.78E+03	10%	(3)
Tellurium	7.78E-01	8.38E-01	1.19E+00	9.37E-01	24%	(2)
Thallium	ND	ND	ND	IDL= 0.414	-	-
Thorium	8.13E+00	8.06E+00	8.36E+00	8.18E+00	10%	(3)
Tin	4.80E+00	4.47E+00	5.62E+00	4.96E+00	12%	(3)
Titanium	3.39E+00	3.38E+00	3.81E+00	3.53E+00	10%	(3)
Uranium	1.19E+02	1.18E+02	1.28E+02	1.22E+02	10%	(3)
Vanadium	1.38E+00	1.22E+00	1.27E+00	1.29E+00	10%	(3)
Zinc	6.84E+01	7.14E+01	7.20E+01	7.06E+01	10%	(3)
Zirconium	3.36E+01	3.13E+01	3.36E+01	3.28E+01	10%	(3)
Chloride	734	753	719	735	NA	(4)
Fluoride	260	212	321	264	NA	(4)
Nitrate	4.17E+05	4.31E+05	3.74E+05	4.08E+05	NA	(4)
Phosphate	ND	ND	ND	MDL= 29	NA	(4)
Sulfate	1.75E+04	7.19E+03	6.31E+03	1.03E+04	NA	(4)

ND Not Detected (detection limit shown in Recommended Value column)
NA Data Not Available
Footnotes:
(1) Uncertainty is calculated within method
(2) Uncertainty is results standard deviation
(3) Uncertainty is the precision shown in the method manual
(4) See discussion in Section 4.5

Table 3-4. WM-189 radionuclide concentrations in liquid from Sample 3 and the Bottom Sample; Units are μCi/L.

Radionuclide	Sample3 Result	Bottom Sample Result	Recommended Value	Value Uncertainty	
Tritium	1.11E+01	8.23E+00	9.67E+00	21%	(1)
Carbon-14	ND	ND	MDA=0.162		
Cobalt-60	5.56E+01	ND	MDA=9.03		
Nickel-59	ND	ND	MDA=3.05E+03		
Nickel-63	ND	1.05E+02	MDA=8.45E+02		
Strontium-90	3.63E+04	4.14E+04	3.88E+04	9%	(1)
Zirconium-95	ND	1.46E+01	MDA=2.48E+04		
Niobium-94	ND	ND	MDA=8.87		
Technetium-99	2.54E+02	2.89E+02	2.72E+02	9%	(1)
Antimony-125	ND	ND	MDA=1.32E+02		
Iodine-129	ND	ND	MDA=3.66		
Cesium-134	4.13E+01	4.03E+01	4.08E+01	11%	(2)
Cesium-137	5.18E+04	4.98E+04	5.08E+04	8%	(2)
Europium-154	1.98E+02	1.75E+02	1.86E+02	10%	(2)
Uranium-234	1.98E+00	1.51E+00	1.75E+00	20%	(2)
Uranium-235	5.47E-02	6.56E-02	6.01E-02	85%	(2)
Uranium-236	6.11E-02	9.52E-02	7.81E-02	75%	(2)
Uranium-238	5.16E-02	3.54E-02	4.35E-02	100%	(2)
Neptunium-237	4.50E-01	4.80E-01	4.65E-01	8%	(2)
Plutonium-238	3.21E+02	4.53E+02	3.87E+02	24%	(1)
Plutonium-239	3.56E+01	5.14E+01	4.35E+01	26%	(1)
Plutonium-241	1.06E+04	1.60E+04	1.33E+04	29%	(1)
Americium-241	6.84E+01	7.84E+01	7.34E+01	15%	(2)
Curium-242	1.38E-02	4.57E-02	2.98E-02	76%	(1)
Curium-244	9.07E-01	1.19E+00	1.05E+00	21%	(2)

ND Not Detected (detection limit shown in Recommended Value column)
NA Data Not Available
Footnotes:
(1) Uncertainty is results standard deviation
(2) Uncertainty is the avg. reported method uncertainty

3.3.2 Solid Phase Analyses

Analytical results for the sludge from the Bottom Sample are reported in Table 3-5. The table was generated similarly to Table 3-3, using raw analytical data from the ALD system. As noted in Section 3.2.2 the sample that was analyzed included TDS from the interstitial liquid as well as UDS in the sludge. Therefore the analytical data is not strictly applicable to the UDS only, but to a blend of UDS and liquid. The portion of the sludge mass that is attributable to the UDS only was estimated in the following way. First, an estimate of the interstitial liquid volume present in the sludge sample, v_i, was obtained from the initial weight of the 15-mL sludge sample (19.562 gm), the final weight of sludge solids obtained after

drying[c] (4.510 gm), the measured density of the Bottoms Sample liquid (1324 gm/L), and the TDS estimated for the liquid under the drying condition applied (250 gm/L)[d].

The following relations were used:

$\nu_i\rho_{liq} + M_{UDS} = 19.562$ gm, and $\nu_i M_{TDS} + M_{UDS} = 4.510$ gm

Solution of these two equations gives the interstitial liquid volume and the mass attributed to the UDS:

$\nu_i = 14.0$ mL

$M_{UDS} = 1.01$ gm

Based on this determination, the UDS constitutes roughly 22 wt% of the total sludge solids after drying (1.01 gm out of 4.510 gm total) and the volume of interstitial liquid per gm of total dried solids is 3.1 mL/gm. In principle this number could be used to calculate the species mass concentrations in the UDS only by subtracting out the TDS portion using ν_i together the measured composition of the liquid. In practice, however, the results from such a procedure would be questionable, given the fact that the TDS constitutes ~80% of the sample that was analyzed, and the uncertainty in the concentrations measured for the liquid portion are generally 10% or higher. The net effect is that the uncertainty in the solids compositions would likely be at least 50%.

Table 3-5. WM-189 non-radioactive species concentrations in sludge from Bottom Sample; Units are mg/kg.

Constituent	Fusion1 Result	Fusion2 Result	Recommended Value	Value Uncertainty	
Aluminum	4.66E+04	4.82E+04	4.74E+04	10%	(2)
Antimony	ND	ND	IDL=43.5		
Arsenic	ND	ND	IDL=36.7		
Barium	1.92E+01	2.33E+01	2.13E+01	14%	(1)
Beryllium	9.62E-01	9.71E-01	9.66E-01	10%	(2)
Boron	6.37E+02	6.94E+02	6.65E+02	10%	(2)
Cadmium	1.04E+03	1.09E+03	1.06E+03	10%	(2)
Calcium	6.99E+03	7.48E+03	7.23E+03	10%	(2)

c. After drying at 125°C per the procedure described in Section 4.2.1.2.

d. The value of 250 gm/L for the UDS was used in place of 295.7 gm/L, which is listed for the Bottom Sample in Table 4-3. The reason is that the sludge solids were dried for a much longer time period than was the liquid sample in the TDS determination (250 hrs vs. 50 hrs). The HSC calculations indicated an asymptotic limit of about 250 gm/L as the molar addition of argon was increased. Since the drying setup was an "open" system, the asymptotic HSC limit was believed to provide a better estimate of the TDS under the conditions used to dry the sludge (see discussion of HSC calculations in Section 4.2.1.2).

Table 3-5. (continued).

Constituent	Fusion1 Result	Fusion2 Result	Recommended Value	Value Uncertainty	
Cerium	ND	ND	IDL=64.5		
Chromium	8.88E+02	7.70E+02	8.29E+02	10%	(1)
Cobalt	7.69E+00	8.74E+00	8.22E+00	10%	(2)
Copper	1.77E+02	1.67E+02	1.72E+02	10%	(2)
Gadolinium	7.52E+01	8.00E+01	7.76E+01	10%	(2)
Gold	ND	ND	IDL=11.7		
Hafnium	ND	ND	IDL=30.2		
Iron	4.75E+03	4.83E+03	4.79E+03	10%	(2)
Lead	5.66E+02	6.07E+02	5.87E+02	10%	(2)
Lithium	1.52E+01	1.25E+01	1.39E+01	14%	(1)
Magnesium	1.11E+03	1.19E+03	1.15E+03	10%	(2)
Manganese	2.55E+03	2.67E+03	2.61E+03	10%	(2)
Molybdenum	9.90E+01	1.02E+02	1.01E+02	10%	(2)
Nickel	4.62E+02	4.16E+02	4.39E+02	10%	(2)
Niobium	2.19E+02	2.30E+02	2.25E+02	10%	(2)
Palladium	ND	ND	IDL=40.4		
Phosphorus	7.89E+03	7.94E+03	7.92E+03	10%	(2)
Potassium	2.82E+04	2.76E+04	2.79E+04	10%	(2)
Ruthenium	1.43E+02	1.21E+02	1.32E+02	12%	(1)
Selenium	ND	ND	IDL=25.9		
Silicon	4.61E+03	4.65E+03	4.63E+03	10%	(2)
Silver	5.66E+01	3.63E+01	4.64E+01	31%	(1)
Sodium	1.59E+05	1.75E+05	1.67E+05	10%	(2)
Strontium	3.90E+01	4.10E+01	4.00E+01	10%	(2)
Sulfur	8.03E+03	8.71E+03	8.37E+03	10%	(2)
Tellurium	ND	ND	IDL=52.7		
Thallium	ND	ND	IDL=44.8		
Thorium	4.29E+01	3.00E+01	3.64E+01	25%	(1)
Tin	1.42E+02	1.35E+02	1.39E+02	10%	(2)
Titanium	6.38E+01	6.80E+01	6.59E+01	10%	(2)
Uranium	3.38E+02	4.74E+02	4.06E+02	24%	(1)
Vanadium	ND	ND	IDL=14.5		
Zinc	2.04E+02	2.35E+02	2.19E+02	10%	(2)
Zirconium	1.09E+04	1.15E+04	1.12E+04	10%	(2)
Chloride	ND	4.23E+02	MDL=0.051	NA	(3)
Fluoride	1.26E+03	2.98E+03	2.12E+03	NA	(3)
Nitrate	4.34E+05	4.13E+05	4.24E+05	NA	(3)
Phosphate	9.20E+03	1.58E+04	1.25E+04	NA	(3)
Sulfate	1.94E+04	1.61E+04	1.77E+04	NA	(3)

ND Not Detected (detection limit shown in Recommended Value column)
NA Data Not Available
Footnotes:
(1) Uncertainty is results standard deviation
(2) Uncertainty is the precision shown in the method manual
(3) See discussion in section 4.5

In addition, it was assumed that in any practical process that might treat the sludge a similar procedure would be used to that used here in obtaining the sludge sample; i.e., the solids would be allowed to settle and the supernatant liquid would be decanted to approximately the top of the stable sludge layer. The sludge slurry would then be pumped out and treated without further separation. For this type of process the compositional information presented here for the sludge slurry is at least approximately applicable. Moreover, it was realized that any *complete* separation of UDS from tank liquid solution would almost certainly require washing of the solids, which (as noted in Ref. 2) would alter the composition of the solids by virtue of the change in the solution with the solids are equilibrated [that solution being the tank fluid prior to washing, and the wash fluid (presumably water) after washing].

Radionuclide concentrations in the sludge were determined and are reported in Table 3-6. Like the chemical composition data in Table 3-5, the radionuclide data is not representative of pure UDS but rather of UDS plus TDS from interstitial liquid.

Table 3-6. WM-189 radioactive species concentrations in sludge from Bottom Sample; Units are μCi/kg.

Radionuclide	Fusion1 Result	Fusion2 Result	Recommended Value	Value Uncertainty	
Tritium	3.50	7.50	5.50	51%	(1)
Carbon-14	ND	ND	MDA=1.03		
Cobalt-60	1.63E+02	1.40E+02	1.51E+02	10%	(1)
Nickel-59	ND	ND	MDA=4.72E+03		
Nickel-63	ND	7.60E+02	MDA=7.00E+02		
Strontium-90	1.02E+05	1.13E+05	1.08E+05	7%	(1)
Zirconium-95	ND	ND	MDA=4.01E+01		
Niobium-94	6.98E+01	9.12E+01	8.05E+01	19%	(1)
Technetium-99	2.93E+03	2.68E+03	2.81E+03	6%	(1)
Antimony-125	ND	ND	MDA=3.00E+02		
Iodine-129	ND	ND	MDA=8.18		
Cesium-134	1.09E+02	1.20E+02	1.15E+02	10%	(2)
Cesium-137	1.31E+05	1.51E+05	1.41E+05	10%	(1)
Europium-154	4.87E+02	5.16E+02	5.02E+02	11%	(2)
Uranium-234	3.83	3.98	3.91	20%	(2)
Uranium-235	1.79E-01	1.01E-01	1.40E-01	47%	(2)
Uranium-236	3.15E-01	2.68E-01	2.92E-01	34%	(2)
Uranium-238	5.96E-02	1.03E-01	8.13E-02	81%	(2)
Neptunium-237	1.48	1.58	1.53	6%	(2)
Plutonium-238	2.26E+03	2.21E+03	2.24E+03	15%	(2)
Plutonium-239	2.58E+02	2.48E+02	2.53E+02	15%	(2)
Plutonium-241	7.94E+04	6.75E+04	7.35E+04	11%	(1)
Americium-241	1.83E+02	1.83E+02	1.83E+02	15%	(2)
Curium-242	2.00E-01	6.48E-02	1.32E-01	72%	(1)
Curium-244	2.64	2.38	2.51	22%	(2)

ND Not Detected (detection limit shown in Recommended Value column)
NA Data Not Available
Footnotes:
(1) Uncertainty is results standard deviation
(2) Uncertainty is the avg. reported method uncertainty

In addition to the analyses described above, SEM EDS analysis (Method 2007) and X-ray diffraction analysis (Method 2702) were performed on the dried sludge sample (UDS+TDS) after it had been dried for ~175 hours at 125°C. Details of these analyses are presented in Appendix B. The principal result of interest reported here was the XRD result that $NaNO_3$ (Nitratine) is the major crystalline component in the dried aggregate solids sample. This result was of interest in identifying a plausible list of compounds present in the dried solids (see Section 4.3). If additional resolution is needed for the composition of UDS *alone* (i.e., after complete separation of the interstitial liquid), this might be accomplished using Transmission Electron Microscope (TEM) technology. This could potentially provide far more detail of tank farm sludge solids structure than XRD technology. TEM microscopy provides crystallographic information at much higher resolution than XRD, and can also provide elemental/compound speciation within the three-dimensional field of view. The INEEL has TEM technology; however, it is not available for analysis of radioactive samples at this time.

A remote Horiba Instruments Model LA-300 (Ref. 6) was utilized to measure the particle size distribution in the analysis on the Bottom Sample sludge sample (see Section 3.2.2). These measured psd's are shown in Figure 3-1; these were performed under non-sonicated conditions.

To provide qualitative information on the agglomeration behavior of WM-189 undissolved solid particles, a drop of the sludge was dispersed in one mL of water. A drop of this dispersion was then placed on a SEM mount and allowed to dry at ambient cell conditions. A photomicrograph of a portion of this dried dispersion is presented in Figure 3-2. This same dispersion technique was performed with isopropyl alcohol; the result is presented in Figure 3-3. The figures indicate that the sludge particle agglomerates were not dispersed, suggesting that the solids are cohesive and likely would require significant measures (e.g., larger volume of dispersing liquid [these dilutions were ~20×; dilution in the Horiba is ~200×] — plus addition of a surfactant, vigorous shear mixing, sonification, etc.) to break up the undispersed particle 'clumps' apparent in the figures.

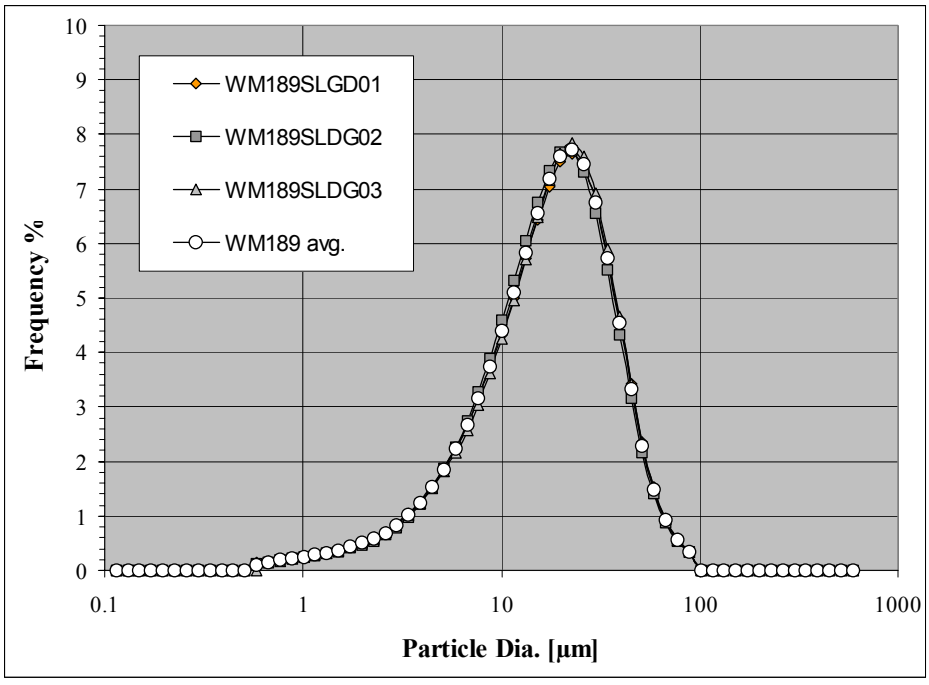

Figure 3-1. WM-189 Sludge Particle Size Distribution Analysis; non-sonicated.

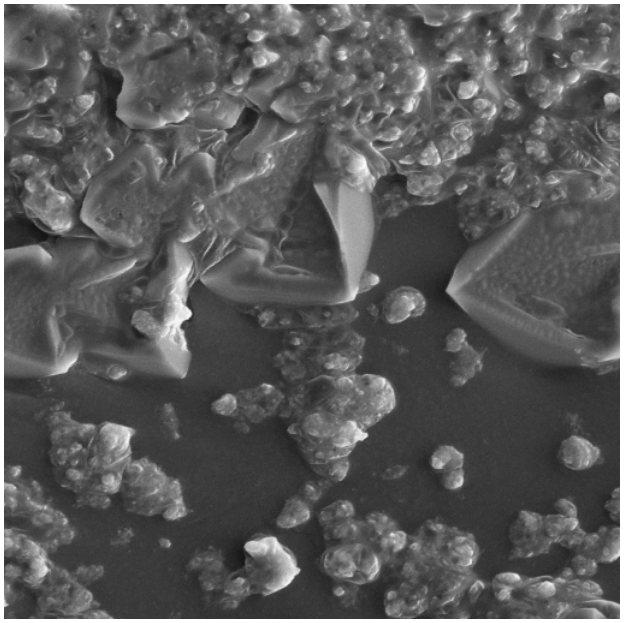

Figure 3-2. SEM photomicrograph of WM-189 sludge dispersed in water; field of view ~92μm wide.

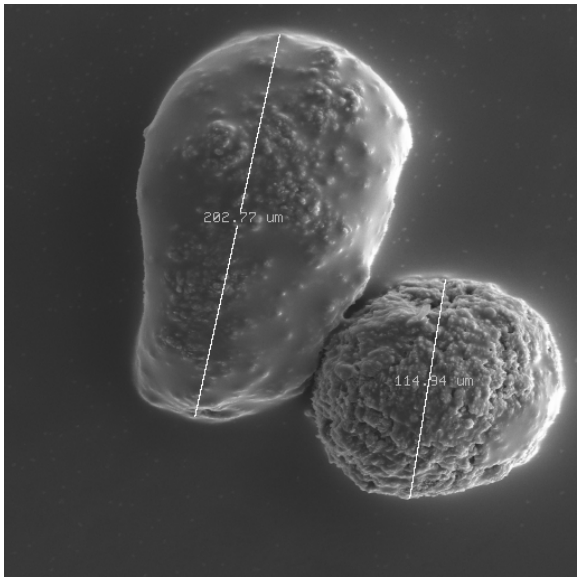

Figure 3-3. SEM photomicrograph of WM-189 sludge dispersed in isopropanol.

Sludge settling rate testing was performed with another ~250 mL portion of 'as received' WM-189 slurry (liquid layer plus sludge layer). The fully agitated condition, and the gravity settled condition of this sample aliquot are shown in Figure 3-4. The settled sludge layer was very light in color and is barely perceptible (in the photo on the right).

Figure 3-4. WM-189 Sludge Sample; fully agitated (l.), gravity settled (r.).

A 25 mL graduated cylinder was used to perform the sludge settling testing. The 250 mL bottle was agitated and 18 mL were delivered to the graduated cylinder. This is shown in Figure 3-5. Three tests were performed. The data for these tests are presented in Appendix B. Test #2 was rerun with shorter time intervals (this constituted the '3rd test'). The results from this testing are presented in Figure 3-6. The settling tests results are discussed further in Section 4.4.4.

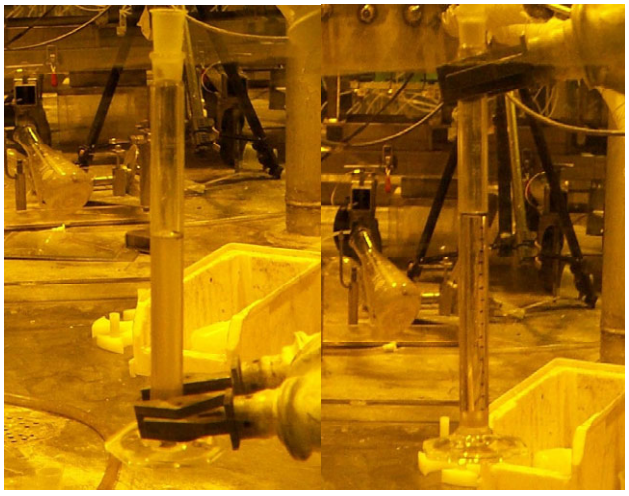

Figure 3-5. WM189 Settling Testing in 25mL Graduated Cylinder; 'time zero'(l.) and settled (r.)

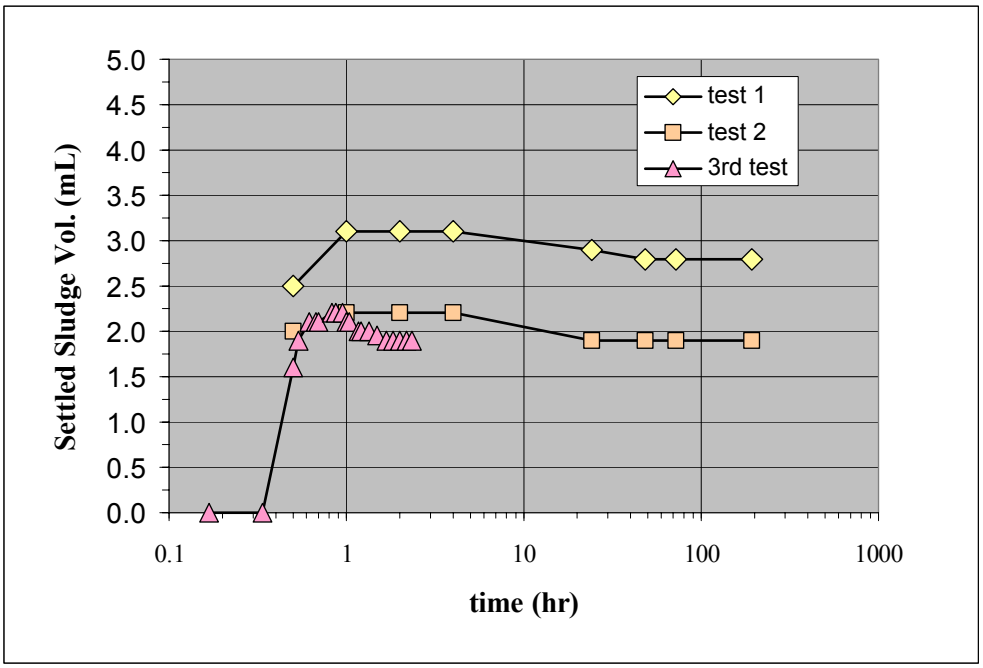

Figure 3-6. Sludge Settling Rate Curve

After completion of the settling rate testing, this slurry material was used for viscosity measurements utilizing the remotized Cole-Parmer Model 98936-00 rotational viscometer located in the RAL hot cell. This viscometer has two spindle/sample cup configurations: 1) a TL-5 spindle in the 8 mL volume 'small sample adapter' cup; and 2) a 'low centipoise' spindle in the 18 mL volume cup. These setups can be operated over eight rotational speeds from 0.3 to 60 rpm. Measurements were taken for the liquid phase, the 'as received' slurry, and the sludge. RAL demin water was used as the reference standard for the liquid and slurry viscosity measurements; water and a Brookfield 50 cP polydimethylsiloxane standard were used for the sludge viscosity measurements.

A corrected viscosity of 1.94 cP (at 30.2°C, 60 rpm) was obtained for the WM-189 liquid phase. WM-189 'as received' slurry and sludge viscosity data are presented in Table 3-7 and Table 3-8, respectively. A viscosity value of 2.6 cP for the 'as received' slurry is in the low end range of the 60 rpm scale. And the 3.5 cP average value for the sludge is below the 5 cP minimum shown on the 60 rpm range. These results are discussed further in Section 4.4.5.

Table 3-7. WM-189 ‘As-Received’ Slurry Viscosity Data

'low centipoise' configuration

			corrected values [cP]		
rpm	Shear Rate [1/sec]	Full Scale [cP]	Test 1	Test 1	Avg. Value
60	73.42	10	2.52	2.73	2.6
30	36.71	20	1.92	2.24	2.1
12	14.68	50	1.47	1.47	1.5
6	7.34	100	3.37	5.27	4.3
3	3.67	200	0.24	0.24	0.2
1.5	1.83	400	0.61	0.62	0.6
0.6	0.73	1,000	0.87	1.09	1.0
0.3	0.36	2,000	—	—	—

Table 3-8. WM-189 Sludge Viscosity Data

TL-5 spindle w/ 8 mL cup configuration

			Standards Reading [cP]		corrected values [cP]			
rpm	Shear Rate [1/sec]	Range [cP]	Demin Water @ 28.2°C: 0.965 cP	Brookfield 50cP @ 28.5°C: 48 cP	Sludge Reading	Sludge/ Water	Sludge/ 50cP Stan	Avg. Value
60	79.20	5-45	15	432	40	2.6	4.4	3.5
30	39.60	10-90	1	443	31	29.9	3.4	16.6
12	15.84	25-225	168	403	67	0.4	8.0	4.2
6	7.92	50-450	271	397	77	0.3	9.3	4.8
3	3.96	100-900	411	295	201	0.5	32.7	16.6
1.5	1.98	200-1.8k	1709	524	54	0.0	4.9	2.5
0.6	0.79	500-4.5k	1923	972	1	0.0	0.0	0.0
0.3	0.40	500-4.5k	6139	1077	1	0.0	0.0	0.0

4. DATA INTERPRETATION

The quality of the analytical data presented in the preceding section is discussed here. Mass balance consistency checks were performed using the gravimetric and analytical measurements to assess the defensibility of the data and the results are presented. WM-189 composition data was also compared with similar data for WM-180. A plausible identification was made of compounds likely to be present in the dried sludge. Finally, uncertainty estimates for anion concentrations (Cl^-, F^-, NO_3^-, PO_4^{-3}, and SO_4^{-2}) are discussed.

4.1 Data Quality

A single quantitative measure of the quality of each data item in the tables in Section 3.3 was provided (where possible) in the form of an overall uncertainty in the last column in the tables. This uncertainty reflects the greater of the analytical method error or the standard deviation between samples when multiple samples were taken.

4.2 Mass Balance Calculations

As a second check on the accuracy of the analytical data for tank liquid and sludge, mass balances were performed by comparing TDS measurements (from weighing dried liquid samples) and dried sludge measurements (from weighing the dried aggregate sludge sample) with the corresponding values obtained by summing the weights of all cations and anions from the chemical analyses of samples. These calculations are described below.

4.2.1 Liquid TDS Mass Balance

4.2.1.1 Baseline. Prior to summing cation and anion masses in the liquid samples, analytical concentrations were adjusted to obtain charge balance in the solution, based on assumed valences listed in Table B-6 of Appendix B. For species with more than one oxidation state, the most stable one was used (from References 7 and 8). This adjustment was done per the following assumptions:

Table 4-1. Assumptions for baseline mass balance calculation.

1	Detection limit values were used for any analyte that *had not* been detected in at least one WM-189 sample, but that *had* been detected in WM-180, per Ref. 2
2	ICP results for sulfur and phosphorous were used to determine sulfate and phosphate concentrations in place of IC results because they were believed to be more accurate (see 4.5 and Ref. 2)
3	Initially assumed valences were changed as follows: Cr^{+3} changed to Cr^{+6}, Zr^{+4} to Zr^{+2}, Hf^{+4} to Hf^{+2}. Stoichiometric amounts of oxygen were then added to convert Cr^{+6} to CrO_4^{-2}, Si to SiO_2 , Zr^{+2} to ZrO, Hf^{+4} to HfO, and U^{+6} to UO_2^{+2} (based on the HSC calculations discussed in Section 4.2.1.2)
4	The NO_3^- concentration was adjusted to eliminate the remaining charge balance [HSC modeling suggests the $Al(NO_3)_3$ aqueous complex over the Al^{+3} cation, justifying an upward adjustment of nitrate value since the IC method (ACMM 8100) only measures free nitrate (Ref. 9)]

Consistent with the reasoning given in Ref. 2 it was assumed that all HNO_3 present in the liquid is volatilized during the drying process. Therefore, in calculating the sum of cation and anion masses H^+ was excluded, together with a stoichiometrically-equivalent quantity of NO_3^-. This sum was compared with the gravimetric TDS measurements (from Table 3-3) for WM-189 Samples 1 and 2, and for WM-180 (as reported in Ref. 2) in Table 3-3. These comparisons and the mass balance results are shown in Table 4-2.

Table 4-2. Baseline TDS mass balance results for WM-189 and WM-180.

Sample	Sum Of Cations and Anions (gm/L)	TDS Measurement (gm/L)	Mass Balance
WM-180	332.2	366.6	91%
WM-189 Sample 1[e]	383.4	290.5	132%
WM-189 Sample 2[e]	382.2	285.0	134%

4.2.1.2 Adjustments to Baseline. The table entries indicate that the TDS mass from the sum of ions exceeds the gravimetric measurement by ~30% for WM-189 calculations. To investigate possible reasons for this discrepancy thermodynamic calculations were performed to identify possible chemical transformations during the drying process prior to the gravimetric measurement. HSC Chemistry® for Windows (Ref. 10) is a thermodynamic equilibrium program that was used for these calculations. The number of moles of all species in the liquid sample which was dried (based on the above assumptions) were provided as input to the program (see Table B-3, Appendix B. Note that Hg, Cr, Cd, Ni, Pb and trace species were not included in the calculation as they were assumed to have negligible impact on the total mass).

HSC calculations assume a closed system. Since the drying procedure was open to the atmosphere, a large molar quantity of argon (Ar) gas was included in the HSC input (Ref. 11) to simulate an open system. Here, "large" means much greater than the total moles in the liquid sample. In principle, this should ensure that the gas phase concentrations of products from the drying process are near zero, as would have been the case in the open system. In practice, it was found that the HSC calculation was sensitive to the quantity of argon assumed, as indicated by the final predicted mass of solids. The quantity of argon was therefore treated as an adjustable parameter to match the final HSC-predicted solids mass to the experimentally-measured value (see following paragraph). Argon was used in place of air in order to prevent HSC from considering N_2 and O_2 in the chemical equilibration. [At 180°C the reactions which equilibrate NO_x with N_2 and O_2 are kinetically slow in comparison with other reactions of interest, notably the decomposition of $Al(NO_3)_3$ to Al_2O_3, which, according to Ref. 12, occurs at approximately 150˚C].

The fact that *all* the drying reactions occur at finite rates means that they are *not* fully equilibrated within the drying time, whereas the HSC equilibrium calculation assumes that they are. In recognition of this, TDS values were redetermined for Samples 1 and 2 and the Bottom Sample at a temperature of 125°C instead of 180°C. In addition, rather than dry for one hour (per ACMM 7004) drying was continued until <5% weight change was observed between sample weighings, which were done roughly once per day. It was assumed that under these conditions all drying reactions simulated by HSC were

e. Dried for 1 hr at 180°C.

100% equilibrated (Refs. 13 and 14. For additional details of the drying procedure see Appendix A). The final TDS values from this procedure are given in column 3 of Table 4-3.

The quantity of argon in the HSC input was adjusted until the predicted total solids mass from the HSC calculation was near the average of the three measured values for WM-189 Samples 1 and 2 and the Bottom Sample in Table 4-3 (~310 g/L).

The speciations predicted from the HSC calculation were used to perform a second mass balance comparing the liquid TDS values from Table 4-3 were compared with the sum of cation and anion masses. This time, however, after applying the assumptions in Table 4-1 a final adjustment to the anion concentrations was done, based on the HSC-predicted speciations during the drying process by HSC (see Table B-4, Appendix B). The only significant difference in speciation from that used for the baseline mass balance was for aluminum. In the former calculation all aluminum was assumed present in the dried solids as $Al(NO_3)_3$, while the HSC calculation indicates 46% of the Al present as $Al(NO_3)_3$ and 54% as Al_2O_3. The results of this second mass balance calculation (along with the WM-180 result presented previously) are given in Table 4-3.

Table 4-3. Adjusted baseline TDS mass balance results for WM-189 and baseline WM-180 result.

Sample	Sum of Cations & Anions (gm/L)	TDS Measurement (gm/L)	Mass Balance
WM-189 Sample 1 (dried @ 125°C)	292.0	328.5	89%
WM-189 Sample 2 (dried @ 125°C)	299.7	306.5	98%
WM-189 Bottom Sample (dried @ 125°C)	288.7	295.7	98%
WM-180 (dried @ 180°C)	332.2	366.6	91%

The Sample 2 and Bottom Sample mass balance results are within 5% of closure. Overall, the results are considered satisfactory. The consistency of the two independent determinations of the dried solids masses from the liquid samples provides a measure of confidence in the accuracy of the analytical data.

4.2.2 Sludge Solids Mass Balance

4.2.2.1 Baseline. An initial mass balance was performed on dried sludge using assumptions 1-3 in Table 4-1 but without assumption 4 (no adjustment for charge imbalance). This yielded a 75.4% mass balance closure (sum of cation/anion masses < gravimetric dried sludge mass) as a baseline.

4.2.2.2 Adjustments to Baseline. As was done for the liquid, the source of the discrepancy in the sludge solids mass balance closure was sought by adjustments to balance charge based on thermodynamic calculations of the probable anions in the dried solids. For the first adjustment it was assumed (from insight provided by the HSC calculations for the liquid) that all the Na^+, K^+, and Al^{+3} are present in the dried sludge solids as $NaNO_3$, KNO_3, $Al(NO_3)_3$, and Al_2O_3, with the Al^{+3} split between $Al(NO_3)_3/Al_2O_3$ using the same 46%/54% split determined from the HSC liquid modeling. The nitrate concentration in the solids based on this assumption was calculated using the measured concentrations of the three cations. The analytically determined nitrate concentration was then replaced with this value with no further adjustments. The resulting mix of cations and anions yielded a net charge imbalance of +0.16 mol/L and a mass balance closure of 99.3% (999.3 mg of cations/anions per gm of sludge solids).

For the second adjustment to the baseline mass balance, the nitrate concentration was further adjusted upward until a charge balance was achieved. The resulting mass balance closure was 100.3%. The near closure with these adjustments supports the validity of the data. It also supports the estimates of the compound breakdown for the sludge solids discussed in Section 4.3.

4.3 Sludge Solids Compounds

On the strength of the above mass balance closure an estimate is provided in Table 4-4 for the compounds that may constitute the bulk of the sludge. The table was obtained as follows. First, a preliminary list of compounds was compiled using the compounds identified as probably constituents of WM-180 solids from Ref. 2. To this list were added the major compounds identified by HSC in the calculation described in Section 4.2.1.2 that were not identified in WM-180 in Ref. 2.

Second, using the analytical data in Table 3-5, the concentrations of Zr, Si, and PO_4^{-3} in TDS from the liquid were compared with their concentrations in the sludge solids. The concentrations in the sludge solids were found to be elevated ~170x, 890x, and 74x, respectively, over their values in the TDS. From this it was inferred that these species were precipitated as UDS from tank liquid. The solid form of the Si was presumed to be SiO_2. Zr and PO_4^{-3} were presumed to have precipitated from the liquid as $Zr(HPO_4)_2$ (Refs. 15, 16, and 17). Based on these assumptions SiO_2 and $Zr(HPO_4)_2$ were added to the preliminary list of compounds. The resulting WM-189 sludge compound list is column 1 of Table 4-4.

Finally, for each compound in the list the analytically-determined concentration of the cation was used to calculate the concentration of the corresponding anion by stoichiometric proportion, from the compound formula. In the case of Al^{+3}, the same 46/54 split between the nitrate and oxide forms was assumed, based on the HSC modeling. The resulting compound concentrations are listed in Table 4-4 as (gm of compound per 100 gm of dried sludge), or wt%. The sum of all species concentrations is 99.4 wt%, indicating that the proposed compound breakdown for the sludge is plausible. The identification of $NaNO_3$ as the major specie in the solids by XRD (see Section 3.3.2) is consistent with Table 4-4, lending additional support to the suggested breakdown.

Table 4-4. Estimated dried sludge compound constituents in WM-189 and WM-180.

Constituent	WM-189 (gm/100 g solids)	WM-180 (gm/100 g solids from Ref. 2)
$NaNO_3$	61.7	28.9
$Al(NO_3)_3$	17.2	25.6
$K_3H_6Al_5(PO_4)_8$	—	12.8
KNO_3	7.21	—
$FePO_4$	—	5.4
Al_2O_3	4.84	—
$Zr(HPO_4)_2$	3.45	—
SiO_2	0.99	4.9
ZrO_2	—	3.7
$AlPO_4$	—	2.8
$CaSO_4$	2.46	—
$Al_2(SO_4)_3$	—	1.8
$Ca(OH)_2 \bullet Ca_3(PO_4)_2$	—	1.0
$MgSO_4$	0.57	—
MnO_2	0.27	—
SnO_2	—	0.27
Fe_2O_3	0.68	—
Mass Balance	**99.4**	**86.9**

An HSC calculation was performed to assess the stability of the WM-189 liquid to precipitation of solids, using the measured composition for the Bottom Sample as input. The calculation predicted precipitation of the following species from the solution at thermodynamic equilibrium: $Al_2(SO_4)_3 \bullet 6H_2O$, KNO_3, $NaNO_3$, K_3AlCl_9, and $Ca(OH)_2 \bullet Ca_3(PO_4)_2$. Since the solution sample is obviously, in fact, stable the prediction is known to be inaccurate. However, it suggests that the indicated compounds may be near saturation in the tank liquid, and thus, may have precipitated earlier. In particular, the presence of KNO_3 and $NaNO_3$ in this list as well as Table 4-4, above, lends additional credence to the claim that they constitute a significant portion of the dried sludge solids.

4.4 Data Comparisons of WM-189 vs. WM-180 and Others

4.4.1 Liquid Phase Chemical and Radiochemistry Data

The liquid phase data from WM-189 and WM-180 SBW is compared in the tables that follow. The liquid phase nonradioactive species molar concentrations (mol/L) and radionuclide activities (Ci/L) are compared in Table 4-5 and Table 4-6, respectively, the last column in each table showing the ratio of WM-189 values to WM-180 values. Cation and anion species are shown in Table 4-5 in order of their concentrations in WM-189. The species order for WM-189 is similar but not identical to that for WM-180. Noteworthy differences in species concentrations that might impact processing requirements are as follows:

- Acid concentration in WM-189 is roughly 3X higher (may have implications on acid gas treatment, corrosion calculation, neutralization processes)
- Hg and Cd concentrations WM-189 are roughly 3X and 5X higher, respectively (may have implications on RCRA disposal of secondary waste streams)
- The Si concentration is about 3 orders of magnitude higher in WM-189. Si is known to scale evaporation equipment, but the concentration is still low in WM-189, ~$3x10^{-4}$ molar.
- Cs concentrations WM-189 are roughly 3X higher (may have implications on required decontamination factors for offgas system components)
- For radionuclides that were analyzed in both WM-189 and WM-180, the WM-189 concentrations are generally higher than those in WM-180. Notable are the ratios for ^{99}Tc, $^{Total}Sr$, ^{134}Cs, ^{137}Cs, and ^{154}Eu, which are ~27X, ~3X, ~5X, ~2X, and ~3X higher respectively in WM-189.

Table 4-5. WM-189 vs. WM-180 liquid phase nonradioactive species comparisons.

Constituent	WM-189 (mol/L)	WM-180 (mol/L)	Ratio 189/180
Acid	2.86E+00	1.01E+00	2.84
Sodium	2.04E+00	2.06E+00	0.99
Aluminum	7.11E-01	6.63E-01	1.07
Potassium	2.25E-01	1.96E-01	1.15
Sulfur	8.58E-02	6.98E-02	1.23
Calcium	7.30E-02	4.72E-02	1.55
Iron	2.68E-02	2.17E-02	1.23
Magnesium	2.21E-02	1.41E-02	1.57
Boron	2.12E-02	1.23E-02	1.72
Manganese	1.95E-02	1.20E-02	1.62

Table 4-5. (continued).

Constituent	WM-189 (mol/L)	WM-180 (mol/L)	Ratio 189/180
Mercury	6.50E-03	2.02E-03	3.22
Chromium	5.64E-03	3.35E-03	1.68
Cadmium	3.91E-03	7.54E-04	5.18
Nickel	2.32E-03	1.47E-03	1.58
Phosphorus	2.07E-03	1.29E-02	0.16
Lead	1.16E-03	1.31E-03	0.89
Zinc	1.07E-03	1.05E-03	1.02
Copper	9.54E-04	6.97E-04	1.37
Hafnium	5.40E-04	-	-
Uranium	5.08E-04	3.36E-04	1.51
Lithium	3.84E-04	3.39E-04	1.13
Zirconium	3.57E-04	6.32E-05	5.64
Silicon	3.08E-04	3.02E-07	1019
Molybdenum	2.80E-04	1.93E-04	1.45
Ruthenium	1.72E-04	1.25E-04	1.38
Strontium	1.41E-04	1.19E-04	1.19
Gadolinium	1.35E-04	1.77E-04	0.76
Titanium	7.30E-05	5.78E-05	1.26
Barium	5.62E-05	5.57E-05	1.01
Cobalt	4.63E-05	1.93E-05	2.40
Tin	4.14E-05	4.11E-05	1.01
Cerium	3.51E-05	-	-
Thorium	3.49E-05	4.73E-05	0.74
Cesium	2.68E-05	7.73E-06	3.46
Vanadium	2.51E-05	9.23E-04	0.03
Beryllium	2.02E-05	7.77E-06	2.60
Antimony	7.52E-06	1.46E-04	0.05
Tellurium	7.26E-06	6.38E-05	0.11
Niobium	IDL=2.49E-07	-	-
Selenium	IDL=4.61E-09	4.99E-04	-
Arsenic	IDL=4.44E-09	1.55E-05	-
Palladium	IDL=3.61E-09	2.35E-05	-
Thallium	IDL=2.03E-09	5.29E-06	-
Silver	IDL=1.87E-09	4.09E-05	-
Nitrate	6.52E+00	5.01E+00	1.30
Sulfate	1.07E-01	5.40E-02	1.98
Chloride	2.06E-02	3.00E-02	0.69
Fluoride	1.38E-02	4.74E-02	0.29
Phosphate	MDL=3.05E-04	1.37E-02	-

Table 4-6. WM-189 vs. WM-180 liquid phase radioactive species comparisons.

Radionuclide	WM-189 Ci/L	WM-180 Ci/L	Ratio 189/180
Tritium	9.66E-06	2.32E-05	0.42
Cobalt-60	MDA=9.03E-06	6.06E-06	-
Total Strontium	3.88E-02	1.35E-02	2.9
Technetium-99	2.71E-04	9.94E-06	27
Iodine-129	MDA=3.66E-06	1.27E-08	-
Cesium-134	4.03E-05	8.80E-06	4.58
Cesium-137	5.01E-02	2.94E-02	1.7
Europium-154	1.84E-04	6.22E-05	2.96
Uranium-234	1.74E-06	1.13E-06	1.54
Uranium-235	6.01E-08	4.18E-08	1.44
Uranium-236	7.81E-08	6.19E-08	1.26
Uranium-238	4.35E-08	2.48E-08	1.75
Neptunium-237	4.59E-07	4.74E-07	0.97
Plutonium-238	3.87E-04	6.39E-04	0.61
Plutonium-239	4.35E-05	9.42E-05	0.46
Americium-241	7.34E-05	8.76E-05	0.84

4.4.2 Solid Phase Chemical and Radiochemistry Data

Sludge data from WM-189 and WM-180 SBW is compared in the tables below. The sludge nonradioactive species concentrations (wt%) and radionuclide activities (Ci/gm) are compared in Table 4-7 and Table 4-8, respectively, with a format similar to the liquid tables above. Cation and anion species are shown in order of their concentrations in WM-189; the order for WM-189 is again similar but not identical to that for WM-180. Noteworthy differences in species concentrations are as follows:

- The concentration of F^- in the WM-189 sludge is 64 times that in WM-180 solids. However, there is no estimate on the F^- uncertainty for the results presented here, so the accuracy of this ratio is uncertain (see Section 4.5).

- The concentrations of ^{239}Pu and ^{238}Pu in WM-180 sludge are ~50X and ~30X their respective values in the WM-189 solids (Note that the WM-189 is *lower* here; in all other bulleted comparisons the WM-189 value is *higher*).

- The concentration of ^{99}Tc WM-189 sludge is ~120X its value in the WM-180 solids.

Table 4-7. WM-189 vs. WM-180 dried solids non-radioactive species concentration (wt%) comparisons.

Constituent	WM-189	WM-180	Ratio 189/180
Sodium	1.67E+01	7.82E+00	2.13
Aluminum	4.74E+00	5.85E+00	0.81
Potassium	2.79E+00	1.47E+00	1.90
Zirconium	1.12E+00	2.80E+00	0.40
Sulfur	8.37E-01	5.06E-01	1.66
Phosphorus	7.92E-01	5.43E+00	0.15
Calcium	7.23E-01	4.30E-01	1.68
Iron	4.79E-01	2.01E+00	0.24
Silicon	4.63E-01	2.09E+00	0.22
Manganese	2.61E-01	1.57E-01	1.67
Magnesium	1.15E-01	1.38E-01	0.83
Cadmium	1.06E-01	1.77E-02	6.01
Chromium	8.29E-02	6.81E-02	1.22
Boron	6.65E-02	-	-
Lead	5.87E-02	5.24E-02	1.12
Nickel	4.39E-02	2.76E-02	1.59
Uranium	4.06E-02	3.48E-02	1.17
Niobium	2.25E-02	-	-
Zinc	2.19E-02	1.96E-02	1.12
Copper	1.72E-02	1.36E-02	1.26
Tin	1.39E-02	2.12E-01	0.07
Ruthenium	1.32E-02	3.59E-02	0.37
Molybdenum	1.01E-02	3.56E-02	0.28
Gadolinium	7.76E-03	8.10E-03	0.96
Titanium	6.59E-03	9.59E-02	0.07
Cerium	IDL=6.45E-03	4.30E-03	-
Tellurium	IDL=5.27E-03	-	-
Silver	4.64E-03	4.90E-03	0.95
Thallium	IDL=4.48E-03	-	-
Antimony	IDL=4.35E-03	4.00E-03	-
Palladium	IDL=4.04E-03	-	-
Strontium	4.00E-03	2.20E-03	1.82
Arsenic	IDL=3.67E-03	-	-
Thorium	3.64E-03	-	-
Hafnium	IDL=3.02E-03	-	-
Selenium	IDL=2.59E-03	-	-
Barium	2.13E-03	3.40E-03	0.63
Vanadium	IDL=1.45E-03	-	-
Lithium	1.39E-03	-	-
Gold	IDL=1.17E-03	-	-
Cobalt	8.22E-04	-	-
Beryllium	9.66E-05	-	-
Nitrate	4.24E+01	4.34E+01	0.98
Sulfate	1.77E+00	8.89E-01	2.00
Phosphate	1.25E+00	6.50E+00	0.19
Fluoride	2.12E-01	3.30E-03	64.13
Chloride	MDL=5.20E-03	9.09E-02	-

Table 4-8. WM-189 vs. WM-180 dried solids radioactive species concentration comparisons.

Radionuclide	WM-189 Ci/g	WM-180 Ci/g	Ratio 189/180
Cobalt-60	1.51E-07	3.55E-08	4.25
Total Strontium	1.08E-04	6.16E-05	1.75
Technetium-99	2.81E-06	2.35E-08	119
Antimony-125	MDA=3.00E-07	3.37E-06	-
Cesium-134	1.15E-07	2.59E-07	0.44
Cesium-137	1.41E-04	2.61E-04	0.54
Europium-154	5.02E-07	4.30E-07	1.17
Uranium-234	3.91E-09	4.31E-09	0.91
Uranium-235	1.40E-10	8.88E-11	1.58
Uranium-236	2.92E-10	1.67E-10	1.75
Uranium-238	8.13E-11	3.79E-11	2.15
Neptunium-237	1.53E-09	3.37E-09	0.45
Plutonium-238	2.24E-06	8.75E-05	0.03
Plutonium-239	2.53E-07	1.30E-05	0.02
Americium-241	1.83E-07	3.13E-07	0.58

4.4.3 Solid Phase Particle Size Distribution

The average WM-189 solids psd is compared to that for WM-180 in Figure 4-1. The WM-180 particles were normally distributed between 2 and 65μm, with both the mode and average size coinciding at 10μm. The WM-189 particles are between 0.5 and 100μm, with the mode and average size coinciding at about 20μm. On this basis the WM-189 solids may be expected to settle considerably faster. These psd's are also compared with the psd's measured for the 1999/2000 WM-182 and –183 LDUA sludge samples (Ref. 18). The Horiba aliquot dispersion/circulation tank has a 13 W, 28 kHz ultrasonic element that can be used to enhance dispersion of particles. However, all psd's presented in Figure 4-1 were performed under non-sonicated condition; a SEM photomicrograph of the WM-182 sludge solids is also presented for comparison with that of WM-189 (see Figure 3-2).

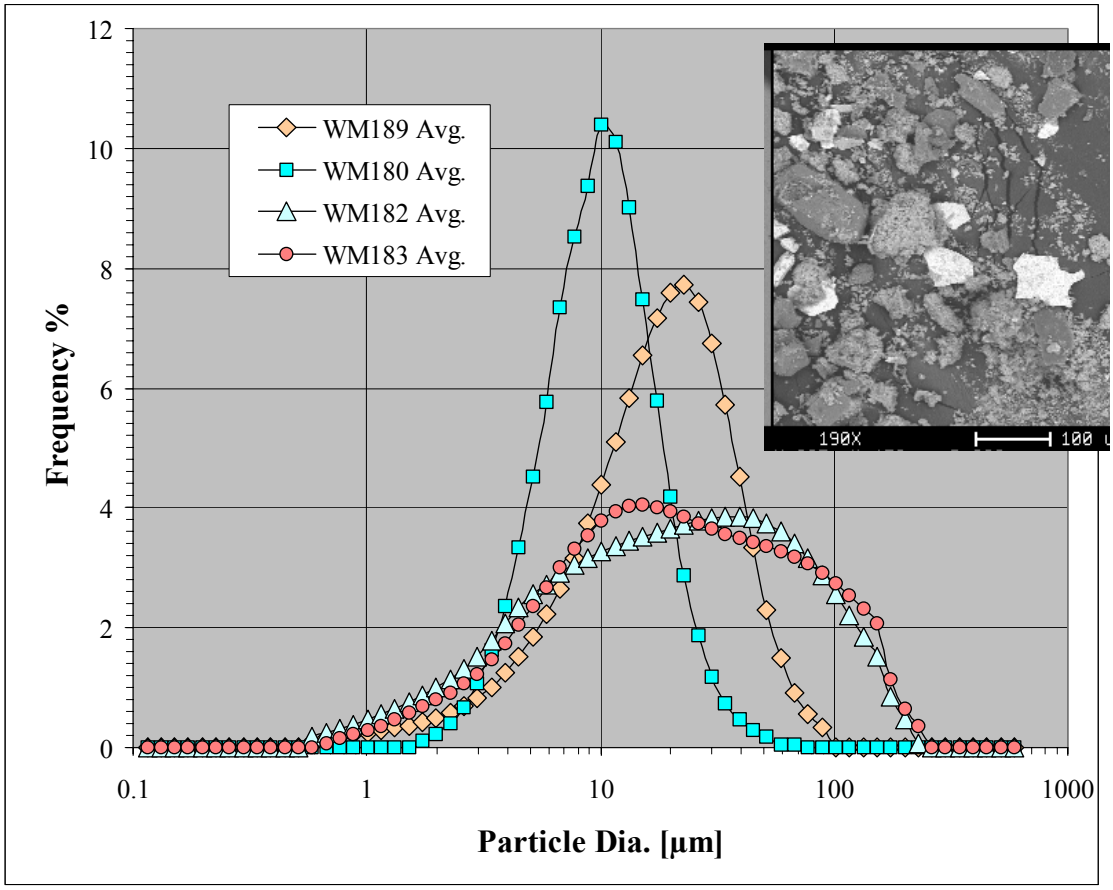

Figure 4-1. Comparison of WM-189 vs. WM-180 (and WM-182,-183 LDUA analyses) solids psd analyses; under non-sonicated condition. SEM photomicrograph of WM-182 solids.

4.4.4 Sludge Settling Testing

WM-189 settling rate testing data was compared against that obtained for the WM-182 LDUA sample (Ref. 19). The WM-189 data was cast in the *settled solids percent* equation as presented by Poloski (in Ref. 19). The WM-189 and -182 data are presented in Appendix B, and a plot of this data is presented in Figure 4-2. With reference to Figure 4-3, Poloski observed a 'slow flocculation sedimentation' regime for the WM-182 sludge. The WM-189 data reflects the upward motion (and then the compression regime of the settled sludge layer) of the sharp interface in the 'accumulation sedimentation' regime (ref. Figure 4-3).

It was concluded that the disparity in 'sludge loading' was the primary factor contributing to the different outcome/observation noted between these two test results. The WM-182 sludge layer was approximately sixty percent of the total sample volume, while the WM-189 sludge layer was only about sixteen percent. The solids also differed greatly in appearance. The WM-182 solids were very dark and nearly opaque, while the WM-189 solids were light gray in color and fairly translucent.

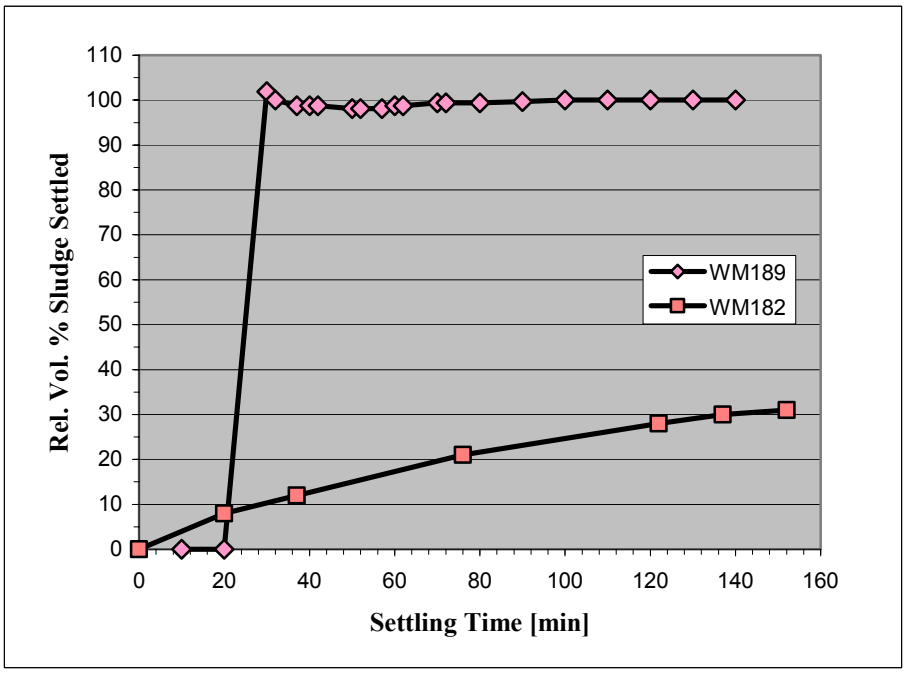

Figure 4-2. WM-189 and WM-182 Rel. Vol. % Settled Sludge vs. Settling Time

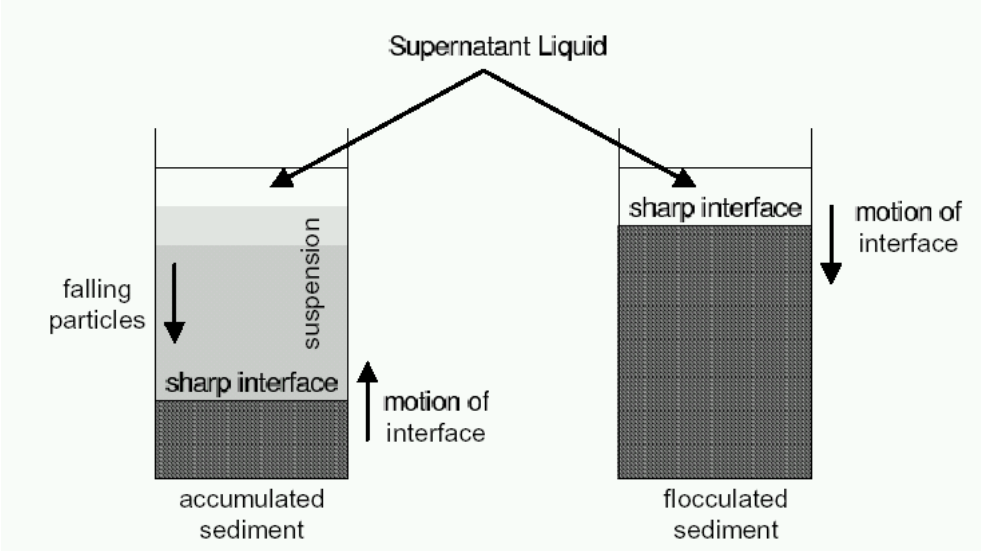

Figure 4-3. Accumulation Sedimentation and Flocculation Sedimentation [see Ref. 19]

4.4.5 Sludge Viscosity Testing

A liquid phase viscosity of 2.2 cP was previously measured for WM-180 (EDF-1914, Ref. 20); this compares with the 1.9 cP measured for WM-189. The average WM-189 sludge viscosity data was compared against that for the WM-182 sludge presented in EDF-1914 (Ref. 20); this comparison is shown in Figure 4-4.

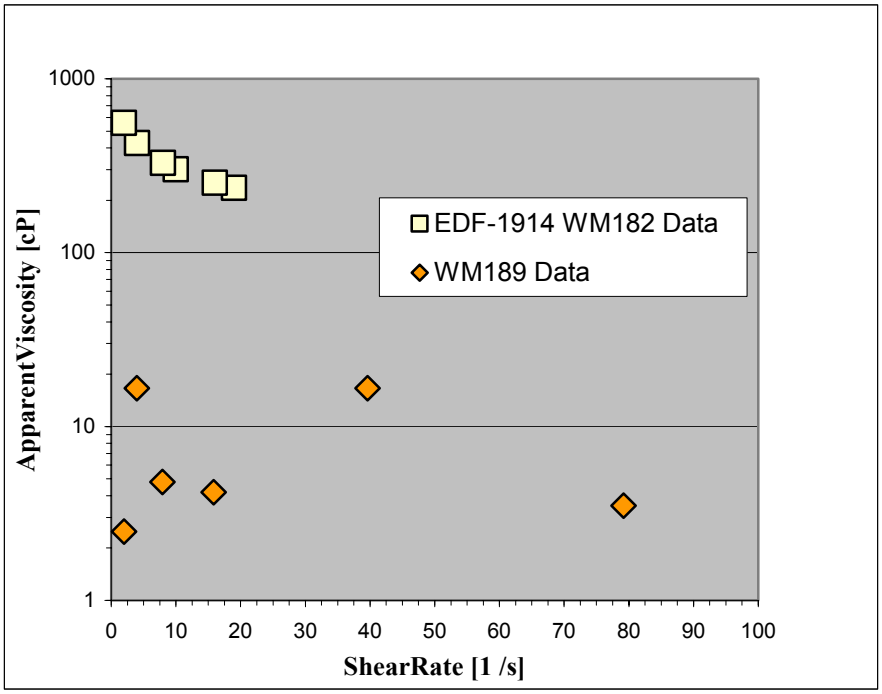

Figure 4-4. WM-182 vs. WM-189 Sludge Viscosity Comparison

The only WM-189 'as received' slurry average corrected viscosity data (in Table 3-7) that fell in the recommended 10 to 90% range (see Cole-Parmer Rotational Viscometers Operation Manual) were at the last upper two shear rates (namely 36.7 and 73.4 [1/s]); the 2.6 cP value was reported. The only WM-189 sludge average corrected viscosity data (in Table 3-8) that fell near (just below) the recommended range was at the upper shear rate, 79.2 (1/s) (the water standard data for the 39.6 (1/s) shear rate was discounted because it did not fit the trend observed in that data). Therefore the 3.5 cP value was reported. In both this WM189 sludge data, and the 'as received' slurry data just discussed, the corrected viscosity values begin to converge/agree at the highest shear rates, indicating that a viscometer configuration with higher shear rate capability is required to obtain acceptably accurate tank heel material viscosity data. Viscometry instrumentation with at least 500 reciprocal seconds shear rate was recommended (Ref. 21).

4.5 Anion Concentration Uncertainties

Concentrations of anions (F^-, Cl^-, NO_3^-, SO_4^{-2}, PO_4^{-3}) were determined by ACMM 8100 (Ion Chromatography), for which no uncertainty is provided by ALD in the published method description (as provided on the Web at http://dune.inel.gov/DeptDocs/Methods/Manual_4/TOC.html). Reasonable estimates for the error were obtained here by (a) comparison of SO_4^{-2} and PO_4^{-3} concentrations with the sulfur and phosphorus measurements from ACMM 2900 (Inductively Coupled Plasma Atomic Emission Spectroscopy), and (b) inferences based on the mass balance closure for the sludge (Table 4-4).

The recommended concentrations of sulfur and phosphorus in the sludge from Table 3-5 were 8,370 mg/kg and 7,920 mg/kg, respectively. Assuming these were 100% speciated as SO_4^{-2} and PO_4^{-3} the equivalent concentrations for the latter would have been 25,100 and 24,300 mg/kg. Based on the compound estimates in Table 4-4, the total concentrations of NO_3^-, SO_4^{-2} and PO_4^{-3} were calculated. The concentrations of the three anions measured by ion chromatography (ACMM 8100) from Table 3-5 were 424,000, 17,700, and 12,500 mg/kg, respectively. A comparison between these results is summarized in Table 4-9.

Table 4-9. WM-189 sludge anion concentrations from analytical methods and from mass balance.

[mg/kg]	ACMM 8100 (IC)	ACMM 2900 (ICP AES)	Table 4-4
NO_3	4.24×10^5	-	6.45×10^5
SO_4	1.77×10^4	2.51×10^4	2.19×10^4
PO_4	1.25×10^4	2.43×10^4	2.33×10^4

There is no spectrometric method for nitrogen, so the only comparison that can be made for nitrate is between the mass balance result and the ion chromatography (ACMM 8100) result. If the mass balance result for nitrate is assumed correct, the ion chromatography number is low by 47%. The initial sludge mass balance discussed in Section 4.2.2.1, based on the analytical results for NO_3^- without adjustment for charge balances, showed ~25% deficiency in the mass balance closure. In addition, there was a large excess of cationic charge over anionic. This, together with the excellent mass balance closure on solids reported in Table 4-4, and the assumption that the IC method measures free nitrate only (Ref. 9), suggests that the above speculation is correct — the nitrate value estimated from the Table 4-4 mass balance is more accurate than that obtained via the ion chromatography method.

With respect to SO_4^{-2} and PO_4^{-3}, Table 4-9 indicates that the emission spectrometry and mass balance (Table 4-4) values differ from the mean of the two values by ~7% and ~2%, respectively, while the ion chromatography values are lower than these mean values by ~33% and ~90%. The consistency between the emission spec and mass balance values suggests they are more accurate and the ion chromatography values are not.

Unfortunately there are no additional measurement methods for the Cl^- and F^- anions other than ion chromatography. Thus, all that can be said is that, based on the other three anion comparisons, the uncertainties in the Cl^- and F^- are likely 25-90%. In general, it appears safe to assume that nominal anion concentrations from ACMM 8100 are low by at least 25%.

5. SIMULANT PREPARATION

Detailed SBW liquid phase simulant preparation instruction/bases were presented in Reference 2. A two liter batch of WM-189 SBW was prepared by L.G. Olson (Ref. 22) utilizing the Reference 2 *SBW simulant solution makeup matrix* spreadsheet. This spreadsheet was prepared specifically for WM-180 simulant, but is valid for any SBW simulant makeup, provided a valid target composition is specified as input (see Section 4.1.2 in Ref. 2). The WM-189 simulant makeup spreadsheet is presented in Figure 5-1.

WM-189 Liquid Simulant Makeup Calculations.
Blue values are numbers entered by the user for the particular situation, if different from the current baseline default values. See notes on NOTES tab worksheet.
Green numbers are derived (floating) values to achieve acid and charge balance.

ENTER VOLUME OF SIMULANT TO PREPARE, IN LITERS: 2

Analyte	Amt of Reagent for 2 Liter(s)	Units	Mol Wt or Conc'n	Units	Form and Notes	Reagent	Moles/L
METALS - BULK ELEMENTAL ANALYSIS							
Aluminum	6.517E-01	Liter	**2.2**	M Al^{3+}	Solution	Al(NO3)3*9H2O	7.168E-01
Arsenic	0.000E+00	g	197.8414	g/mol		As2O3	0.000E+00
Arsenic	0.000E+00	g	389.7985	g/mol	Alternate Arsenic acid	H5As3O10[a]	0.000E+00
Barium	3.136E-02	g	261.3398	g/mol		Ba(NO3)2	6.000E-05
Beryllium	0.000E+00	g	47.00898	g/mol		BeF2	0.000E+00
Boron	2.549E+00	g	61.83302	g/mol		H3BO3	2.061E-02
Cadmium	2.418E+00	g	308.48092	g/mol		Cd(NO3)2*4H2O	3.920E-03
Calcium	3.458E+01	g	236.14892	g/mol		Ca(NO3)2*4H2O	7.322E-02
Cerium	2.605E-02	g	434.22638	g/mol		Ce(NO3)3*6H2O	3.000E-05
Chromium	3.799E+00	g	328.0871	g/mol		Cr(NO3)3*5H2O	5.790E-03
Cobalt	2.910E-02	g	291.03468	g/mol		Co(NO3)2*6H2O	5.000E-05
Copper	4.735E-01	g	241.60164	g/mol		Cu(NO3)2*3H2O	9.800E-04
Gadolinium	1.213E-01	g	433.3411	g/mol		Gd(NO3)3*5H2O	1.400E-04
Iron	2.173E+01	g	403.99922	g/mol		Fe(NO3)3*9H2O	2.689E-02
Lead	7.684E-01	g	331.2098	g/mol		Pb(NO3)2	1.160E-03
Lithium	5.102E-02	g	68.9459	g/mol		LiNO3	3.700E-04
Magnesium	1.126E+01	g	256.40648	g/mol		Mg(NO3)2*6H2O	2.195E-02
Manganese	1.393E+01	g solution	178.9478	g/mol	AlfaAesar50% soln	Mn(NO3)2	1.946E-02
Mercury	4.200E+00	g	342.61508	g/mol		Hg(NO3)2*H2O	6.130E-03
Molybdenum	5.600E-03	Liter	**0.1**	M MoO2(NO3)2[b]	Soln:see prep notes	Mo in HNO3	2.800E-04
Nickel	1.349E+00	g	290.79488	g/mol		Ni(NO3)2*6H2O	2.320E-03
Potassium	4.482E+01	g	101.1032	g/mol		KNO3	2.217E-01
Ruthenium	0.000E+00	g	207.4281	g/mol		RuCl3	0.000E+00
Ruthenium	0.000E+00	Liter	**1.48E-01**	molar solution	Alternate:Solution of	Ru(NO)(NO3)3[c]	0.000E+00
Ruthenium	0.000E+00	g	237.434	g/mol	2nd Alternate for Ru	Ru(NO)Cl3[d]	0.000E+00
Sodium	3.540E+02	g	84.99467	g/mol		NaNO3	2.082E+00
Strontium	5.926E-02	g	211.6298	g/mol		Sr(NO3)2	1.400E-04
Titanium	0.000E+00	g	189.6908	g/mol		TiCl4	0.000E+00
Uranium	0.000E+00	g	502.12928	g/mol		UO2(NO3)2*6H2O	0.000E+00
Zinc	6.366E-01	g	297.49148	g/mol		Zn(NO3)2*6H2O	1.070E-03
Zinc	0.000E+00	g	136.2954	g/mol	Alternate: ZnCl2	ZnCl2[e]	0.000E+00
Zirconium	1.440E-03	Liter	**0.5**	M ZrF4 in 3.0M HF[f]	Soln:see prep notes	ZrF4	3.600E-04
ANION ANALYSES							
Chloride	3.497E-03	Liter	**12**	molar solution		HCl	2.098E-02
Fluoride	7.100E-04	Liter	**28.9**	molar solution		HF[g]	1.026E-02
Fluoride	0.00000	g	**48**	wt% HBF4 solution	Alternate for F	HBF4[g]	0.000E+00
Iodide	4.313E-02	g	166.0028	g/mol		KI	1.299E-04
Nitrate	3.442E-01	Liter	**15.4**	molar solution		HNO3	2.651E+00
Phosphate	2.959E-04	Liter	**14.6**	molar solution		H3PO4	2.160E-03
Sulfate	9.411E-03	Liter	**18**	molar solution		H2SO4	8.470E-02
RADIONUCLIDE ANALYSES AND SIMULANTS.[h]							
TOTAL ELEMENTAL CONCENTRATION CALCULATED FROM RADIONUCLIDE ANALYSES.							
Cesium	1.169E-02	g	194.91035	g/mol		CsNO3	3.000E-05
Cesium	1.010E-02	g	168.3582	g/mol	Alternate: CsCl	CsCl	3.000E-05
Europium	0.000E+00	g	446.0705	g/mol		Eu(NO3)3*6H2O	0.000E+00
Rhenium[i]	0.000E+00	Liter	**0.00537**	M Re, 0.814MHNO3	Aqueous solution of	Re in 5% HNO3	0.000E+00
Neodymium[j]	0.000E+00	g	438.346			Nd(NO3)3*6H2O	0.000E+00
Thorium[k]	0.000E+00	Liter	**0.00431**	M Th, 0.814MHNO3	Aqueous solution of	Th(NO3)4 in 5% HNO3	0.000E+00
ELEMENTS LOOKED FOR BUT NOT DETECTED[l]							
CONCENTRATIONS GIVEN ARE DETECTION LIMITS EXCEPT WHEN INDICATED AS A CALCULATED LIMIT THAT IS LESS THAN THE DETECTION LIMIT. IF ANY OF THESE IS NOT ADDED, ENTER ZERO IN ITS RESPECTIVE CELL IN ROW 70 TO ELIMINATE THE SMALL EFFECT ON CALCULATED ANION CONCENTRATIONS. NOTE VALUE DELETED FOR FUTURE.							
Antimony	0.000E+00	g	228.115			SbCl3	0.000E+00
Niobium (Calcd)	0.000E+00	Liter	**0.01076**	M Nb, 0.998 M HF	Aqueous solution of	NbCl5 in 2% HF	0.000E+00
Palladium	0.000E+00	g solution[m]	**8.5**	wt% Pd=7.99E-4 mol/g solution.	Solution	Pd(NO3)2	0.000E+00
Selenium	0.000E+00	Liter	**0.01266**	M Se, 0.814MHNO3	Aqueous solution of	Se in 5% HNO3	0.000E+00
Silicon	0.000E+00	Liter	**0.03561**	M Si, 0.814MHNO3	Aqueous solution of	Si in 5% HNO3	0.000E+00
Silver	0.000E+00	g	169.873			AgNO3	0.000E+00
Thallium	0.000E+00	Liter	**0.004893**	M Tl, 0.814MHNO3	Aqueous solution of	Tl in 5% HNO3	0.000E+00
Tin (Calcd)[n]	0.000E+00	g	156.7068			SnF2	0.000E+00
Vanadium	0.000E+00	Liter	**0.01963**	M V, 0.814MHNO3	Aqueous solution of	V in 5% HNO3	0.000E+00

Figure 5-1. WM-189 Simulant MakeUp Spreadsheet.

A clear, stable WM-189 simulant solution was obtained for process development and laboratory testing purposes.

6. CONCLUSIONS AND RECOMMENDATIONS

1. WM-189 liquid and sludge samples were obtained from near the 10 ft level and from the bottom of the tank. The compositions of these samples were measured in terms of chemical and radioactive constituents and quantitative measures of the uncertainties in the data were provided.

2. Concentrations of anions typical of INTEC TFF wastes (F^-, Cl^-, NO_3^-, SO_4^{-2}, PO_4^{-3}) were measured using ACMM 8100 (ion chromatography). Large uncertainties in the reported values for NO_3^-, SO_4^{-2}, PO_4^{-3} were identified and similar uncertainties are likely in the values for F^- and Cl^-. In light of the role of these latter species in material corrosion and process air emissions limits it is recommended that more reliable methods be investigated for measuring their concentrations.

3. Satisfactory liquid TDS mass balance closure was achieved using the WM-189 SBW liquid phase data reported here; thus the analytical data is considered appropriate for SBW process modeling purposes. The Tier 2 liquid phase data, in conjunction with the information in this report could be used to support permitting.

4. Satisfactory mass balance closure was also achieved for solids derived from drying of WM-189 sludge using the analytical data for the sludge reported here.

5. No definitive insight was acquired for the sludge solids from SEM EDS analysis data. The INEEL has microprobe technology that could provide superior elemental analysis, especially for nitrogen and oxygen. Further investigation of the possibility of applying this technology and/or TEM technology to tank farm sludge characterization is recommended.

6. Comparison of WM-189 and WM-180 compositions show significant differences for the following constituent concentrations: H^+, Hg, Cd, Cs, Si, ^{99}Tc, $^{Total}Sr$, ^{134}Cs, ^{137}Cs, and ^{154}Eu.

7. A clear, stable WM-189 simulant solution was prepared utilizing the *SBW simulant solution makeup matrix* spreadsheet. This WM-189 SBW simulant is considered suitable for laboratory testing purposes.

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Appendix A

Supporting Documents for 2002 WM-189 Sampling

WM-189 Sampling Activity Summary

14-Mar-02

The *SBW Characterization* Work Package WM-189 sampling activities have been completed. Three airlift samples, and a single steam jetted "bottom sample" have been acquired for characterization analyses.

In preparation for these sampling activities, three ~300 gal. flushes of WM-189 solution were transferred through NCC-101 late Friday, 8 Mar 2002, to early Saturday morning; this is shown, along with the sampling events, in Figure 1. Approximately 1,000 gal. were then transferred into NCC-101 and "sample 1" was drawn under fully sparged conditions (late Sunday night —see Fig. 1). This solution was transferred out and another ~1,000 gal. brought in Monday afternoon; "sample 2" was drawn late Monday night. Similarly, "sample 3" was obtained late Tuesday night.

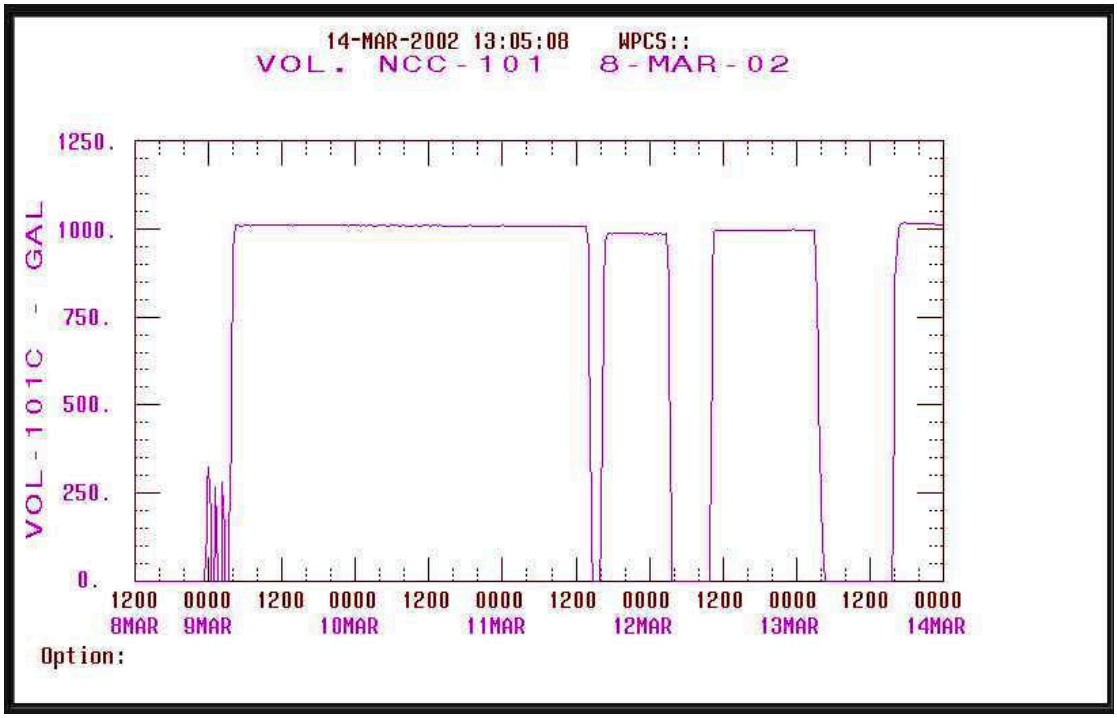

Figure 1. NCC-101 WM-189 sampling activities.

Specific gravity (SpGr) measurements (per ACCM 7981) were determined for these samples. An 'outlier' rejection test was used to determine if these samples were from a statistically similar solution.

$$B_4 = \frac{SpGr_{\max} - SpGr_{\min}}{\sigma}$$

SpGr analysis is chosen because it provides the quickest analysis turn-around, and is a reasonably precise and accurate method. SpGr data has traditionally been used in INTEC nuclear material accountability and fuel storage sampling processes. Also, SpGr will be used in the thermodynamic modeling calculations of the SBW. The SpGr data results for these samples are presented in Figure 2.

Originally, the SpGr method standard deviation, σ , was used in the outlier test. It was realized that this was too "tight" (conservative) a restriction on the data. A less restrictive approach was taken by calculating the standard deviation from the triplicate test data for each of the samples — and then using the average sample standard deviation in the outlier test. Just as in the original approach, the result indicated that "sample 3" was statistically different (lower) than "sample 1" and "sample 2"; these results are shown in Figure 3. A liberal approach was then taken where the standard deviation from all of the SpGr data was used with the range of the entire data set; this result is also presented in Figure 3. This approach indicated that "sample 3" need not be rejected; this was too liberal. This juncture was reached late Wednesday (13 Mar). Based on these results, this investigator would preferred to have taken another upper stage airlift sample—"sample 4", to clarify the data trend. However the decision to 'not draw this sample' was made. Instead, it was decided to draw the "bottom sample" using the WM-189 steam-jet; this sample was obtained late Wednesday night. Unfortunately, this sample can not be presently transferred to the RAL because the receiving manipulator at RAL is broken; it may not be functional until late next week. So, as it turns out, if "sample 4" (a RCRA protocol sample…same as samples one through three) had been taken, its protocol hold times would probably have been exceeded.

	SpGr data	σ	Sample Avg.	Sample stan dev	Avg. σ	Avg. Sample σ	Avg. Sample stan dev
Sample 1	1.33574	7.9E-04	1.33501	1.32E-03	7.9E-04	7.76E-04	1.56E-03
	1.33349	7.8E-04					
	1.33581	7.9E-04					
Sample 2	1.33300	7.80E-04	1.33315	3.37E-04	7.8E-04		
	1.33292	7.80E-04					
	1.33354	7.80E-04					
Sample 3	1.32450	7.60E-04	1.32257	3.01E-03	7.6E-04		
	1.32412	7.60E-04					
	1.31910	7.60E-04					

Figure 2. WM-189 upper airlift stage sample SpGr data.

Some of the filled "bottom sample" bottles were inspected this morning (14 Mar) at NWCF. A very gelatinous white mass of settled solids was observed in each bottle inspected. Upon gently tilting the bottle, the mass deformed slightly, but remained as a plug. Upon slight/gentle agitation, the solids dispersed quite freely — and the dispersion appeared to be less translucent than was observed in the pre-agitated condition.

Also this morning, a "one factor analysis of variance " was performed for the airlift SpGr data. The *Data Analysis/Anova: Single Factor* option under the Tools menu in EXCEL® was utilized. These results are presented in Figure 4; these results also indicated that a "sample 4" should probably have been taken to perhaps clarify the data trend. These results were independently validated by Dr. Ivan Thomas (INEEL Safeguards and Personnel Security).

Per original approach, use SpGr method σ as divisor on range (most conservative)

B_4 = 16.04

16.04 >> 3.31

B_4 is much greater than the Table10.3 value (3.31 @ 5% level, n=3),
therefore reject the lower 1.32257 SpGr sample - and take fourth sample

A 'middle' approach, use avg. sample stan deviation as divisor on range

B_4 = 7.99

7.99 > 3.31

B_4 is still greater than the Table10.3 value (3.31 @ 5% level, n=3),
therefore reject the lower 1.32257 SpGr sample - and take fourth sample

Use all data (n=9)...and use data standeviation for divisor (most liberal)

Column1	
Mean	1.330246667
Standard Error	0.00201394
Median	1.333
Mode	#N/A
Standard Deviation	0.006041819
Sample Variance	3.65036E-05
Kurtosis	-0.522432046
Skewness	-0.988799417
Range	0.01671
Minimum	1.3191
Maximum	1.33581
Sum	11.97222
Count	9

B_4 = Range / data stan dev = 2.77

2.77 < 4.39

B_4 is less than Table10.3 value (4.39@ 5% level, n=9),
therefore do not reject sample 3 - perform analyses with these three samples

Figure 3. Outlier test results.

WM-189 Sample SpGr Data

ANOVA: One Factor Analysis of Varience (with Tools/Data Analysis/Anova: Single Factor)

Sample 1	Sample 2	Sample 3
1.33574	1.33300	1.32450
1.33349	1.33292	1.32412
1.33581	1.33354	1.31910

Anova: Single Factor (with all three samples)

SUMMARY

Groups	*Count*	*Sum*	*Average*	*Variance*
Column 1	3	4.00504	1.335013	1.74E-06
Column 2	3	3.99946	1.333153	1.14E-07
Column 3	3	3.96772	1.322573	9.08E-06

ANOVA

Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
Between Groups	0.00027	2	0.000135	37.04231	0.000421	5.143249
Within Groups	2.19E-05	6	3.65E-06			
Total	0.000292	8				

F > F crit …that is, 37.04 > 5.1432: samples may ~~not~~ be from an identical population.

Anova: Single Factor (with samples 1 and 2 only)

SUMMARY

Groups	*Count*	*Sum*	*Average*	*Variance*
Column 1	3	4.00504	1.335013	1.74E-06
Column 2	3	3.99946	1.333153	1.14E-07

ANOVA

Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
Between Groups	5.19E-06	1	5.19E-06	5.593935	0.077228	7.70865
Within Groups	3.71E-06	4	9.28E-07			
Total	8.9E-06	5				

F < F crit …that is, 5.59 < 7.71: these samples (samples one and two) are probably from an identical population.

Figure 4. EXCEL Anova: One Factor Analysis of SpGr data.

WM-189 TDS @ 125°C

Date Modified: 11-Aug-02

Avg. TDS (g/litre) = 317.53

	TDS Mass (gram)					DryTime (hr)	Preparation Description
Sample	Gross	Tare	Net	% change	TDS (g/l)		
Sample 1	52.49725	38.65387	13.84338		1384.3	0	10.0 ml of sample liquid, 16-May-02
	-	-	-	-		-	evap down on hotplate @ 95°C on 20-May-02
	42.07362		3.41975		342.0	24	mass after 1st 125°C; overnite oven-drying; 8:30, 21-May-02
	42.00787		3.35400	1.9%	335.4	29.5	mass after more 125°C drying; 14:00, 21-May-02
	41.93912		3.28525	2.0%	328.5	53.5	mass after 2nd overnite @ 125°C oven-drying; 8:30, 22-May-02
Sample 2	52.61937	39.06000	13.55937		1355.9	0	10.0 ml of sample liquid, 16-May-02
	-	-	-	-		-	evap down on hotplate @ 95°C on 20-May-02
	42.40225		3.34225		334.2	24	mass after 1st 125°C; overnite oven-drying; 8:30, 21-May-02
	42.27788		3.21788	3.7%	321.8	29.5	mass after more 125°C drying; 14:00, 21-May-02
	42.12537		3.06537	4.7%	306.5	53.5	mass after 2nd overnite @ 125°C oven-drying; 8:30, 22-May-02
Bottom Sample	52.49788	39.14425	13.35363		1335.4	0	10.0 ml of sample liquid, 16-May-02
	-	-	-	-		-	evap down on hotplate @ 95°C on 20-May-02
	42.63625		3.49200		349.2	24	mass after 1st 125°C; overnite oven-drying; 8:30, 21-May-02
	42.49663		3.35238	4.0%	335.2	29.5	mass after more 125°C drying; 14:00, 21-May-02
	42.10137		2.95712	11.8%	295.7	53.5	mass after 2nd overnite @ 125°C oven-drying; 8:30, 22-May-02

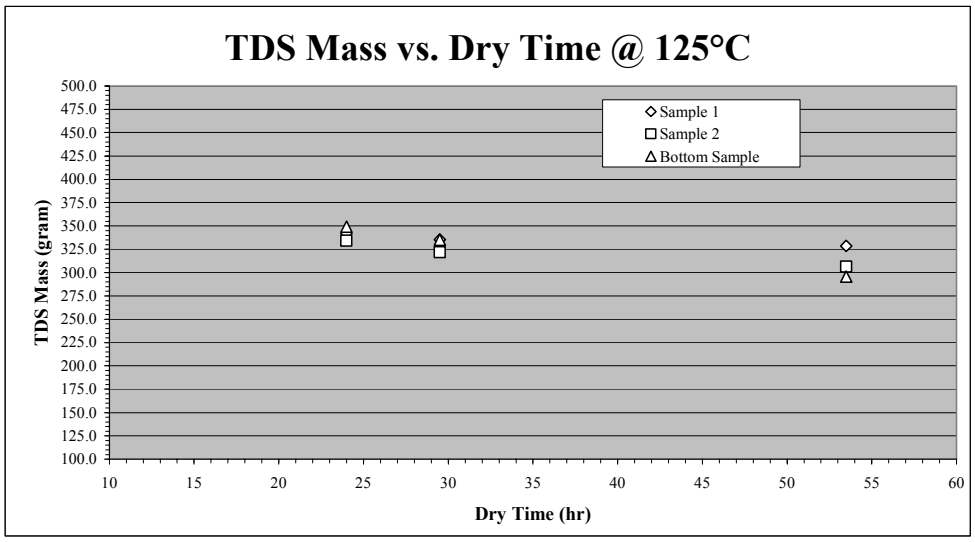

Figure A-1. WM-189 TDS Experimental Procedure Details.

Sludge Mass (gram)			DryTime (hr)	Preparation Description
Gross	Tare	Net		
52.69888	33.13700	19.56188	0	15.0 ml separated liquid sludge in tared centrifuge tube
-	-	-	-	transferred sludge to Pt crucible
67.86938	49.72300	18.14638	72	sludge dried in RAL cell over weekend @ 85°F; weighed 6-May-02
59.97662		10.25362	88	mass after 1st 95°C evaporation; 7-May-02
59.45938		9.73638	104	mass after 2nd 95°C evaporation; 7-May-02
58.59488		8.87188	106	mass after 1st 115°C/~2hr oven-drying; 7-May-02
58.54825		8.82525	108	mass after 2nd 115°C/~2hr oven-drying; 8-May-02
56.53725		6.81425	122	mass after 1st 125°C; overnite oven-drying; 9-May-02
56.50962		6.78662	184	mass after 3-day weekend; lost power to oven, air dry only; 13-May-02
54.65275		4.92975	208	mass after 2nd 125°C; overnite oven-drying; 14-May-02
54.29400		4.57100	232	mass after 3rd 125°C; overnite oven-drying; 15-May-02
broke-up solids in Pt crucible with spatula on 15-May-02 A.M. (after initial weighing). Pre-break-up mass 54.290875 g; post-break-up mass 54.288625; assume 0.00225 g lost on spatula.				
-	-	4.56850	232	mass remaining after solids break-up step; 15-May-02
54.23300		4.51000	256	mass after 4th 125°C; overnite oven-drying; 16-May-02
this last weighing was only a 1.3% weight loss - therefore, these dried UDS were nearly ready the fusion analyses. These solids were transfered from the Pt crucible to a poly bottle, and were pulverized/"homogenized" with a glass rod. The $\rho_{dried\text{-}UDS}$ was determined using a graduated glass cylinder - $\rho_{dried\ UDS} = 1.13$. Since approx. 1/2 g was 'encrusted' on the Pt crucible, there remains only about 4 g of pulverized/oven-dried UDS...this material will be used for the fusion analyses and SEM EDS 14:30, 16-May-2002 - TAB.				

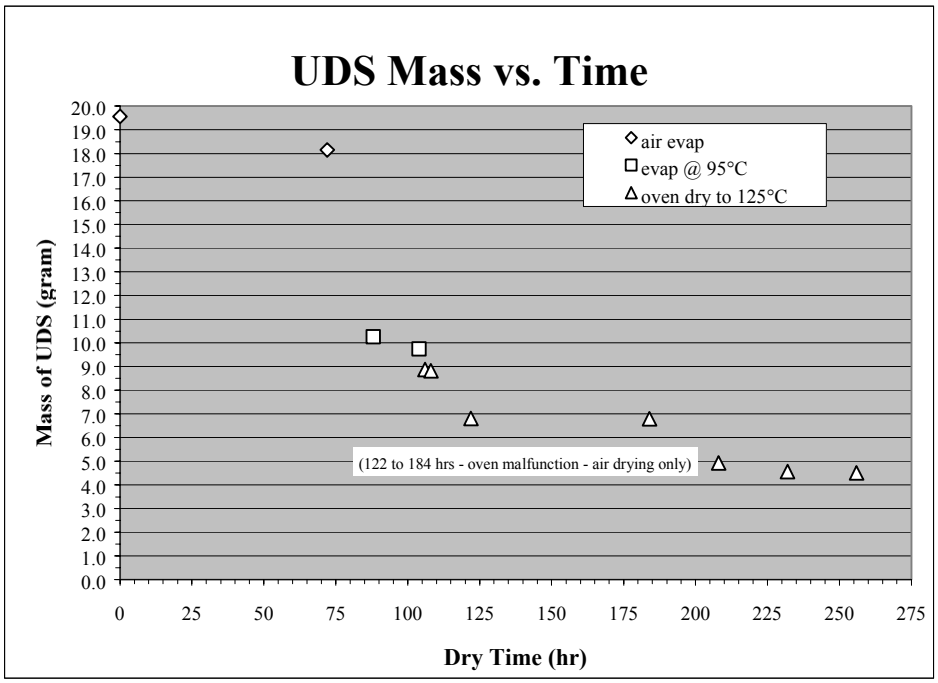

Figure A-2. WM-189 Bottom Sample Sludge Preparation for Fusion Analyses.

Appendix B

Additional Data From 2002 WM-189 Sampling

Table B-1. Volatile Organic Compound Analyses 'Hit' Data; from Tier2 Report.

all organic data in μg/L

Organic Compound	Sample 1	LQF	Sample 2	LQF	Sample 2 (re-ran)	LQF	Sample 2 Avg.	BottomSample	LQF	Bottom Sample w/ 2.8% dilution	Samples' Avg. Value	%RSD
Chloromethane	23	M	35	M			35	75	HM	77	45	63%
Bromomethane	13	B	32	B			32	59	H	61	35	68%
Acetone	33	BY	11	BY	6	JBY	8.5				21	83%
Tentatively Identified VOC's												
Unknown (4.80 min)								11	JH	11	11	-
Unknown (4.85 min)	6	J									6	-
Unknown (4.92 min)								6	JH	6	6	-
Unknown (16.17 min)	17	J						8	JH	8	13	49%
Unknown (17.0 min)			16	J			16				16	-
Unknown (17.07 min)	8	J						120	JH	123	66	124%
Unknown (33.02 min)								16	JH	16	16	-
VOA (TOTAL) [mg/L]	**0.10**						**9.2E-02**			**0.30**	**0.16**	**73%**

LQF (Laboratory Qualifier Flag)

M = quantified from first or higher order regression fit calibration curve w/ correlation coefficient <0.999

J = estimated (extrapolated) value

H = hold time exceeded

B = analyte also detected in blank

Y = analyte is also a solvent used in hot cell for other methods

Table B-2. SemiVolatile Organic Compound Analyses 'Hit' Data; from Tier2 Report.

all organic data in [µg/L]

Organic Compound	Sample 1	LQF	Sample1 (re-ran)	LQF	Sample 1 avg.	Sample 2	LQF	Bottom Sample	LQF	Bottom Sample w/ 2.8% dilution	Samples' Avg. Value	%RSD
Isophorone								82	H	84	84	-
Dibenzofuran								12	JH	12	12	-
Tri-n-butyl phosphate	11	BJM	11	BJM	11	11	BJM	44	H	45	22	88%
bis(2-Ethylhexyl)phthalate	46	M	31	M	39			25	H	26	32	28%
Di-n-octylphthalate	20		16	J	18						18	-
Tentatively Identified SVOC's												
Unknown (6:27 min)								29	JH	30	30	-
Unknown (7:25 min)								130	JH	134	134	-
Unknown9 (7:34 min)	21	J	15	J	18	36	J				27	47%
Unknown Hydrocarbon 1 (7:49 min)						18	BJM				18	-
Unknown (8:23 min)								74	JH	76	76	-
Unknown Hydrocarbon 3 (8:29 min)						12					12	-
Unknown10 (13:58 min)	89	J	70	J	80	94	J				87	12%
Unknown20 (15:50 min)						33	J				33	-
Unknown (16:06 min)								240	JH	247	247	-
Unknown (16:12 min)								42	JH	43	43	-
Unknown (16:41min)								150	JH	154	154	-
Unknown (16:53min)								64	JH	66	66	-
Unknown (17:07min)								78	JH	80	80	-
Unknown (17:18 min)								89	JH	91	91	-
Unknown (17:23 min)								44	JH	45	45	-
Unknown (17:35 min)								150	JH	154	154	-
Unknown (17:56 min)								120	JH	123	123	-
Unknown (18:04 min)								110	JH	113	113	-
Unknown (18:18 min)								110	JH	113	113	-
Unknown (18:21 min)								71	JH	73	73	-
Unknown (18:50 min)								41	JH	42	42	-
Unknown (19:02 min)								40	JH	41	41	-
Unknown (19:10 min)								60	JH	62	62	-

Table B-2. (continued).

Tentatively Identified SVOC's	Sample 1	LQF	Sample1 (re-ran)	LQF	Sample 1 avg.	Sample 2	LQF	Bottom Sample	LQF	Bottom Sample w/ 2.8% dilution	Samples' Avg. Value	%RSD
Unknown (19:39 min)								120	JH	123	123	-
Unknown (20:26 min)								65	JH	67	67	-
Unknown Phthalate Ester1 (30:00 min)	35	J			35						35	-
Unknown Phthalate Ester2 (30:12 min)	20	J			20						20	-
Unknown Phthalate Ester3 (30:17 min)	43	J	30	J	37						37	-
Unknown14 (30:22 min)	22	J	14	J	18						18	-
Unknown Phthalate Ester4 (30:27 min)	56	J	37	J	47						47	-
Unknown Phthalate Ester5 (30:37 min)	39	J	27	J	33						33	-
Unknown Phthalate Ester6 (30:47 min)	35	J	21	J	28						28	-
Unknown Phthalate Ester7 (30:52 min)	45	J	27	J	36						36	-
Unknown Phthalate Ester8 (31:02 min)	81	J	56	J	69						69	-
Unknown Phthalate Ester9 (31:07 min)	117	J	78	J	98						98	-
Unknown15 (31:14 min)	45	J	33	J	39						39	-
Unknown16 (31:18 min)	66	J	41	J	54						54	-
Unknown Phthalate Ester10 (31:24 min)	112	J	74	J	93						93	-
Unknown Phthalate Ester11 (31:35 min)	28	J	19	J	24						24	-
Unknown Phthalate Ester12 (31:41 min)	49	J	36	J	43						43	-
Unknown Phthalate Ester13 (31:48 min)	73	J	50	J	62						62	-
Unknown Phthalate Ester14 (31:58 min)	70	J	49	J	60						60	-
Unknown Phthalate Ester16 (36:48 min)			17	J	17						17	-
Unknown 2 (38:20 min)	50	BJ	33	BJ	42	33	BJ				37	16%
SVOA (TOTAL) [mg/L]					**1.0**	**0.24**				**2.0**	**1.1**	**83%**

LQF (Laboratory Qualifier Flag)

M = quantified from first or higher order regression fit calibration curve w/ correlation coefficient <0.999

J = estimated (extrapolated) value

H = hold time exceeded

B = analyte also detected in blank

WM-189 Settling Rate Testing

time [hr]	Vol Settled [ml] test#1	test#2
0.5	2.5	2
1	3.1	2.2
2	3.1	2.2
4	3.1	2.2
24	2.9	1.9
48	2.8	1.9
72	2.8	1.9
192	2.8	1.9

WM189 3rd Test (shorter time intervals)

Time	Minutes	Hours	mL's Settled	Vol. % Settled	Comments
1448	0		0	0	cloudy
1458	10	0.167	0	0	cloudy
1508	20	0.333	0	0	cloudy
1518	30	0.500	1.6	102	particles agglomerating @1515
1520	32	0.533	1.9	100	slanted accumulation
1525	37	0.617	2.1	99	
1528	40	0.667	2.1	99	
1530	42	0.700	2.1	99	
1538	50	0.833	2.2	98	
1540	52	0.867	2.2	98	
1545	57	0.950	2.2	98	Mostly clear
1548	60	1.000	2.1	99	Solution clear 1/16 cloudy above
1550	62	1.033	2.1	99	solids
1558	70	1.167	2	99	" " " " "
1600	72	1.200	2	99	" " " " "
1608	80	1.333	2	99	" " " " "
1618	90	1.500	1.95	100	" " " " "
1628	100	1.667	1.9	100	Clear
1638	110	1.833	1.9	100	Clear
1648	120	2.000	1.9	100	Clear
1658	130	2.167	1.9	100	Clear
1708	140	2.333	1.9	100	Clear

log 0203131

Semi-quant analysis for Air dried sample.

Air-p1-1 (Air dried sample, particle 1, spectrum 1)

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	31.31	53.52	1.44	0.89	0.2541	5916.7
Na ?	4.53	5.39	1.02	3.58	0.0189	728.5
Al	27.87	28.25	1.10	1.10	0.1788	7931.2
K ?	9.82	6.87	1.03	1.24	0.0770	2810.8
Ca ?	3.89	2.66	0.91	2.18	0.0311	1078.8
Nb ?	1.17	0.34	0.37	5.13	0.0091	268.6
Au ?	21.41	2.97	1.04	1.93	0.1589	3540.8
Total	100.00					

? The presence of these elements is questionable.

Air-p1-2

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	33.27	52.67	1.56	0.55	0.3056	17973.9
Na ?	8.75	9.64	1.13	1.62	0.0369	2590.7
Al	27.02	25.36	0.89	0.66	0.1676	14438.2
K	10.61	6.87	1.08	0.64	0.0857	6279.6
Ca ?	4.48	2.83	0.82	1.12	0.0365	2555.1
Nb ?	4.06	1.11	0.77	1.55	0.0312	1864.3
Au ?	11.80	1.52	1.04	1.69	0.0863	3897.7
Total	100.00					

? The presence of these elements is questionable.

Air-p1-3

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	32.08	50.94	1.31	0.45	0.2754	21905.9
Na ?	14.31	15.81	0.66	0.98	0.0623	7172.3
Al	24.75	23.30	0.90	0.58	0.1465	20413.7
K	7.99	5.19	1.09	0.62	0.0637	7314.8
Ca ?	2.96	1.88	0.67	1.13	0.0242	2640.2
Nb ?	3.95	1.08	0.83	1.31	0.0302	2829.0
Au ?	13.95	1.80	0.64	1.32	0.1020	7200.0
Total	100.00					

? The presence of these elements is questionable.

Air-p1-4

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	28.28	53.91	1.33	0.88	0.1941	6035.9
Na ?	0.00	0.00	0.00	3.30	0.0000	0.2
Al	23.69	26.77	1.03	1.04	0.1546	10160.1
K ?	13.03	10.16	0.73	1.02	0.1004	5332.6
Ca ?	5.26	4.00	1.09	1.82	0.0408	2056.6
Nb ?	3.17	1.04	0.84	2.73	0.0258	1107.3
Au ?	26.56	4.11	1.15	1.68	0.2063	6680.7
Total	100.00					

? The presence of these elements is questionable.

Figure B-1. SEM EDS Results on WM-189 ‘air-dried’ TDS material.

Oven Dried

Thursday, April 25, 2002 4:08:22 PM
Ovn-p1-1

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	36.24	50.10	1.43	0.81	0.2168	6295.6
Na	25.15	24.19	1.12	1.06	0.1160	5968.3
Al	24.62	20.18	1.07	0.90	0.1322	8047.1
K	4.36	2.47	0.99	1.04	0.0362	1750.4
Ca ?	2.43	1.34	0.68	1.51	0.0211	965.1
Nb ?	7.20	1.72	1.15	1.37	0.0523	2056.1
Au ?	0.00	0.00	0.00	2.57	0.0000	0.2
Total	100.00					

? The presence of these elements is questionable.

Thursday, April 25, 2002 4:11:38 PM
Ovn-p1-2

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	33.40	47.68	1.36	1.08	0.1883	5278.3
Na	29.07	28.88	1.20	1.28	0.1342	7132.9
Al ?	18.94	16.03	0.96	1.36	0.0978	6025.2
K	6.69	3.91	1.14	1.12	0.0554	2692.3
Ca ?	2.43	1.38	0.70	2.01	0.0207	954.0
Nb ?	7.80	1.92	1.12	1.67	0.0584	2334.5
Au ?	1.67	0.19	0.55	7.82	0.0119	358.3
Total	100.00					

? The presence of these elements is questionable.

Thursday, April 25, 2002 4:12:29 PM
Ovn-p1-3

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	36.59	52.26	1.37	1.13	0.1845	4923.3
Na ?	17.97	17.86	1.00	1.55	0.0786	4197.6
Al	25.91	21.95	1.13	1.06	0.1479	8926.5
K	6.87	4.02	1.13	1.09	0.0565	2696.7
Ca ?	2.76	1.57	0.79	1.87	0.0234	1060.2
Nb ?	9.20	2.26	0.94	1.52	0.0681	2678.7
Au ?	0.69	0.08	0.27	12.98	0.0049	144.6
Total	100.00					

? The presence of these elements is questionable.

Thursday, April 25, 2002 4:13:21 PM
Ovn-p2-4

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	32.37	48.02	1.37	0.84	0.2302	6168.2
Na ?	27.49	28.39	1.17	1.26	0.1278	5904.5
Al ?	19.98	17.58	0.96	1.22	0.1057	5828.4
K ?	4.14	2.51	0.96	1.38	0.0333	1460.4
Ca ?	1.53	0.91	0.47	2.36	0.0129	536.2
Nb ?	6.26	1.60	1.15	1.74	0.0471	1690.5
Au ?	8.23	0.99	1.15	3.29	0.0592	1596.8
Total	100.00					

? The presence of these elements is questionable.

Figure B-2. SEM EDS Results on WM-189 180ºC ‘oven-dried’ TDS material.

Thursday, May 23, 2002 3:59:18 PM
Uds-p1-1

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	30.58	41.16	2.41	1.40	0.2968	1430.1
Na	47.96	44.93	1.77	1.45	0.2538	1425.4
Al ?	11.11	8.87	1.30	3.58	0.0487	403.2
S ?	0.99	0.66	0.31	6.68	0.0069	57.0
K ?	5.62	3.09	1.13	2.83	0.0484	302.2
Ca ?	1.35	0.73	0.41	5.84	0.0120	71.3
Zr ?	2.39	0.56	0.67	6.80	0.0166	86.6
Total	100.00					

? The presence of these elements is questionable.

Thursday, May 23, 2002 4:01:07 PM
Uds-p2-2

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	34.45	47.84	2.31	1.29	0.2741	2040.4
Na ?	21.63	20.91	1.18	1.89	0.0988	874.9
Al ?	25.07	20.64	1.17	1.83	0.1391	1609.3
S ?	0.09	0.06	0.04	18.33	0.0006	8.1
K ?	15.37	8.73	0.82	1.47	0.1348	1254.4
Ca ?	3.22	1.78	0.77	3.73	0.0272	244.4
Zr ?	0.18	0.04	0.08	21.38	0.0012	9.7
Total	100.00					

? The presence of these elements is questionable.

Thursday, May 23, 2002 4:01:56 PM
Uds-p3-3

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	35.62	47.69	2.37	1.18	0.3107	1992.4
Na	31.21	29.09	1.47	1.52	0.1518	1085.3
Al ?	21.51	17.08	1.12	2.04	0.1094	1077.4
S ?	2.04	1.36	0.55	4.08	0.0143	142.6
K ?	6.14	3.37	1.15	2.32	0.0525	408.4
Ca ?	2.00	1.07	0.54	4.20	0.0175	129.4
Zr ?	1.47	0.35	0.45	7.53	0.0101	65.4
Total	100.00					

? The presence of these elements is questionable.

NOTE: Uds-p4-4 was not quantified because it was collected as a point spectrum on a particle high in Zirconium and so it was not representative of the solids in general.

Thursday, May 23, 2002 4:03:09 PM
Uds-p5-5

Element	Wt. Pct.	At. Pct.	Std. Dev.	MDL	k-Ratio	Intensities
O	31.41	42.24	2.27	1.33	0.2854	1636.9
Na	44.35	41.50	1.68	1.38	0.2309	1652.1
Al ?	13.75	10.96	0.93	2.99	0.0622	631.7
S ?	0.80	0.54	0.27	7.08	0.0057	56.5
K ?	6.35	3.49	1.19	2.48	0.0548	426.9
Ca ?	1.58	0.85	0.47	5.10	0.0140	103.1
Zr ?	1.76	0.42	0.54	7.51	0.0122	78.6
Total	100.00					

? The presence of these elements is questionable.

Figure B-3. SEM EDS Results on WM-189 125°C cured UDS Material.

Bechtel BWXT Idaho, LLC

ANALYTICAL CHEMISTRY
SPECTROCHEMICAL ANALYSIS

Record No.	02-D-7	Log No.	0203141
Analyzed By	BRB	Project	WM-189 sludge
Approved By		Charge No.	562B32221
Sample Activity	none	Requested By	Tom Batcheller
Method	SEM/XRD	Page Number	1 of 1

Sample Name	X-ray Diffraction Results
Oven Dried	$NaNO_3$ (Nitratine)is the major crystalline component of this sample. Amorphous material is present. Due to the small sample size, unidentified crystalline material is probably present.

Figure B-4. XRD Analysis Results for 125°C dried WM-189 UDS material.

Table B-3. HSC WM-189 INPUT Deck

	A	B	C	D
1	**Species Formula**	INPUT (mols)	phase mol%	
2	**Gases**	0.001	100.000	
3	Ar(g)	0.001	100.000	
4	Cl2(g)			
5	ClO3F(g)			
6	HCl(g)			
7	HF(g)			
8	HNO3(g)			
9	H2O(g)			
10	H2S(g)			
11	NO(g)			
12	NO2(g)			
13	N2O4(g)			
14	**Fluorides, etc.**	0.000	100.000	
15	AlF3	0.000	100.000	
16	B3O3F3			
17	CaF2			
18	**Chlorides, etc.**	0.000	100.000	
19	CaCl2	0.000	100.000	
20	CaCl2*4H2O			
21	CaCl2*6H2O			
22	Ca(ClO3)2			
23	Ca(ClO4)2			
24	FeCl2			
25	FeCl3			
26	FeCl2*2H2O			
27	FeCl2*4H2O			
28	K3AlCl9			
29	MgCl2*H2O			
30	MgCl2*2H2O			
31	MgCl2*4H2O			
32	MgCl2*6H2O			
33	MnCl2*2H2O			
34	MnCl2*4H2O			

Table B-3. (continued).

	A	B	C	D
35	**Oxides, etc.**	0.000	100.000	
36	Al4B2O9	0.000	100.000	
37	Al18B4O33			
38	Al(NO3)3*6H2O			
39	Al2O3			
40	Al2O3(C)			
41	Al2O3(D)			
42	Al2O3(G)			
43	Al2O3(K)			
44	Al2O3*H2O			
45	Al2O3*H2O(B)			
46	Al2O3*3H2O			
47	Al2(SO4)3			
48	Al2(SO4)3*6H2O			
49	B2O3			
50	B2O3(A)			
51	B2O3(G)			
52	Ca(NO3)2			
53	Ca(NO3)2*2H2O			
54	Ca(NO3)2*3H2O			
55	Ca(NO3)2*4H2O			
56	CaO			
57	CaO*Al2O3			
58	CaO*2Al2O3			
59	*2CaO*Al2O3			
60	*3CaO*Al2O3			
61	*12CaO*7Al2O3			
62	*3CaO*Al2O3*6H2O			
63	*4CaO*Al2O3*13H2O			
64	*2CaO*Fe2O3			
65	Ca(OH)2*Ca3(PO4)2			
66	CaSO3			
67	CaSO4			
68	CaSO4(A)			
69	CaSO4(B)			
70	CaSO3*0.5H2O			
71	CaSO3*2H2O			
72	CaSO4*0.5H2O			
73	CaSO4*0.5H2O(A)			
74	CaSO4*0.5H2O(B)			
75	CaSO4*2H2O			

Table B-3. (continued).

	A	B	C	D
76	**Oxides, etc.(cont.)**			
77	Fe2MgO4			
78	Fe2MnO4			
79	FeO			
80	FeO1.5(W)			
81	Fe2O3			
82	Fe2O3(H)			
83	Fe3O4			
84	Fe3O4(H)			
85	Fe2O3*H2O			
86	FeO*OH			
87	FeSO4			
88	Fe2(SO4)3			
89	FeSO4*H2O			
90	FeSO4*4H2O			
91	FeSO4*7H2O			
92	HBO2			
93	H3BO2			
94	H3BO3			
95	HNO3			
96	H2SO4			
97	H2SO4*3H2O			
98	H2SO4*4H2O			
99	KNO3			
100	Mg(NO3)2			
101	Mg(NO3)2*6H2O			
102	MgO			
103	MgO(M)			
104	MgO2			
105	MgO*Al2O3			
106	MgSO3			
107	MgSO4			
108	MgSO4(A)			
109	MgSO4(B)			
110	MgSO4*H2O			
111	MgSO4*2H2O			
112	MgSO4*4H2O			
113	MgSO4*6H2O			
114	MgSO4*7H2O			
115	Mn(NO3)2			
116	MnO			
117	MnO2			
118	Mn2O3			
119	Mn3O4			
120	MnO*Al2O3			
121	MnO*Fe2O3			
122	MnSO4			
123	MnSO4*H2O			
124	MnSO4*4H2O			
125	MnSO4*5H2O			
126	MnSO4*7H2O			
127	NaNO2			
128	NaNO3			

Table B-3. (continued).

	A	B	C	D
129	**Elements**	0.000	100.000	
130	FeB	1.00E-36	100.000	
131	Fe2B			
132	**Aqueous**	56.293	100.000	
133	H2O	42.550	75.586	
134	Al(+3a)	0.722	1.283	
135	Al(NO3)3(a)			
136	AlO(+a)			
137	Ar(a)			
138	H3BO3(a)	0.021	0.037	
139	BO2(-a)			
140	Ca(+2a)	0.074	0.131	
141	Cl(-a)	0.021	0.037	
142	F(-a)	0.014	0.025	
143	Fe(+3a)	0.027	0.048	
144	Fe(+2a)			
145	FeCl2(+a)			
146	FeF(+2a)			
147	H(+a)	2.925	5.196	
148	HF(a)			
149	HNO3(a)			
150	HNO2(a)			
151	H2S(a)			
152	K(+a)	0.220	0.391	
153	Mg(+2a)	0.022	0.039	
154	MgCl(+a)			
155	MgSO4(a)			
156	Mn(+3a)	0.020	0.036	
157	Mn(+2a)			
158	N2(a)			
159	NH4(+a)			
160	NO3(-a)	7.511	13.342	
161	Na(+a)	2.079	3.693	
162	NaNO3(ia)			
163	NaCl(a)			
164	O2(a)			
165	OH(a)			
166	OH(-a)			
167	PO4(-3a)	0.002	0.004	
168	SO4(-2a)	0.085	0.152	

Table B-4. WM-189 25ºC Solution Stability HSC OUTPUT

C:\My Documents\TAB HSC Folder\TAB HSC Calc\WM189liq2.OGI					
Date: 15 Aug 2002/18:00			**Data: 1**		
	Phase	**MW g/mol**	**Temperature: 25°C**		
			[mol]	(liq) [mol/litre]	(s) [g/l]
H2O(g)	1	18.015	1.00E-36		
H2O	6	18.015	4.24E+01		
O2(a)	6	31.999	3.41E-02		
NO3(-a)	6	62.005	3.25E+00	3.2532	
H(+a)	6	1.007	2.48E+00	2.4812	
NaNO3(ia)	6	84.995	1.65E+00	1.6516	
N2(a)	6	28.013	8.61E-03		
HNO3(a)	6	63.013	4.46E-01	0.4464	
HNO3(g)	1	63.013	1.00E-36		
NO2(g)	1	46.006	1.00E-36		
Al(NO3)3(a)	6	212.996	6.61E-01	0.6610	
Na(+a)	6	22.989	3.96E-01	0.3956	
K(+a)	6	39.098	8.94E-02	0.0894	
KNO3	4	101.103	1.24E-01		12.50
Al2O3*H2O	4	119.976	1.77E-22		0.00
Al2O3(C)	4	101.961	2.55E-26		
Ca(+2a)	6	40.079	6.78E-02	0.0678	
Al2O3	4	101.961	2.15E-26		
NaNO3	4	84.995	3.18E-02		2.70
Al2O3*H2O(B)	4	119.976	2.83E-24		
Al2(SO4)3*6H2O	4	450.227	2.85E-02		12.81
Mg(+2a)	6	24.304	2.20E-02	0.0220	
H3BO2	4	45.833	2.09E-02		0.96
MnO2	4	86.937	2.34E-03		0.20
Mn(+2a)	6	54.937	1.77E-02	0.0177	
MgSO4(A)	4	120.363	1.36E-05		0.00
FeF(+2a)	6	74.844	1.40E-02	0.0140	
Fe(+3a)	6	55.845	1.30E-02	0.0130	
Al2O3(K)	4	101.961	8.51E-28		
Al(+3a)	6	26.980	1.75E-03	0.0017	
Al2O3(D)	4	101.961	5.99E-28		
MgSO4(B)	4	120.363	2.89E-06		0.00
Fe2O3	4	159.692	1.53E-08		0.00
Al4B2O9	4	273.541	1.00E-36		
FeO*OH	4	88.854	1.99E-05		0.00
HBO2	4	43.817	3.99E-05		0.00
K3AlCl9	3	463.353	2.33E-03		1.08
Ca(NO3)2	4	164.090	5.80E-07		
Ca(NO3)2*4H2O	4	236.151	1.53E-03		0.36
CaSO4	4	136.138	7.11E-08		
HF(g)	1	20.006	1.00E-36		
Ca(OH)2*Ca3(PO4)2	4	384.277	1.07E-03		0.41
Ar(a)	6	39.948	1.00E-03		
Ar(g)	1	39.948	1.00E-36		
Al2O3(G)	4	101.961	1.51E-29		

Table B-4. (continued).

H3BO3(a)	6	61.832	1.90E-05	0.0000	
HNO3	4	63.013	1.06E-05		0.00
FeCl2(+a)	6	126.752	2.86E-06	0.0000	
Ca(NO3)2*3H2O	4	218.135	3.18E-04		0.07
Fe2O3*H2O	4	177.707	2.99E-09		
CaSO4(A)	4	136.138	3.00E-09		
FeO1.5(W)	4	79.846	7.38E-10		
CaSO4*0.5H2O(B)	4	145.145	1.17E-08		
NO(g)	1	30.006	1.00E-36		
CaSO4*0.5H2O(A)	4	145.145	1.73E-08		
CaSO4*0.5H2O	4	145.145	1.50E-08		
CaSO4(B)	4	136.138	4.24E-10		
Ca(NO3)2*2H2O	4	200.120	4.37E-05		0.01
N2O4(g)	1	92.011	1.00E-36		
HF(a)	6	20.006	5.55E-11	0.0000	
H3BO3	4	61.832	3.67E-06		0.00
Mg(NO3)2*6H2O	4	256.406	1.14E-05		0.00
Mn(+3a)	6	54.936	6.17E-06		
AlO(+a)	6	42.980	1.25E-14		
Al2O3*3H2O	4	156.007	1.07E-23		
CaSO4*2H2O	4	172.168	7.84E-08		0.00
HCl(g)	1	36.461	1.00E-36		
NaCl(a)	6	58.443	7.48E-11		
Cl(-a)	6	35.454	1.06E-09		
Fe(+2a)	6	55.846	3.44E-11		
Al18B4O33	4	1056.888	1.00E-36		
F(-a)	6	18.999	4.69E-14		
HNO2(a)	6	47.013	4.41E-11		
B2O3	4	69.618	2.05E-16		
MgCl(+a)	6	59.757	1.68E-11		
MgSO4(a)	6	120.363	1.42E-09		
MgSO4*H2O	4	138.378	1.46E-12		
Mn2O3	4	157.874	5.15E-15		
Al(NO3)3*6H2O	4	321.087	1.36E-09		
B2O3(A)	4	69.618	2.34E-18		
B2O3(G)	4	69.618	2.17E-18		
MnSO4*H2O	4	169.011	1.88E-12		
MnO*Al2O3	4	172.899	1.00E-36		
MgSO4	4	120.363	1.59E-17		
Mg(NO3)2	4	148.315	4.30E-17		
SO4(-2a)	6	96.059	2.23E-10		
NaNO2	4	68.995	2.04E-16		
MnSO4	4	150.996	2.10E-15		
H2SO4*4H2O	4	170.134	9.23E-12		
MgSO4*7H2O	4	246.469	6.39E-11		
Mn(NO3)2	4	178.948	7.02E-15		
H2SO4*3H2O	4	152.119	1.65E-12		
MgSO4*6H2O	4	228.454	3.07E-11		
Cl2(g)	1	70.906	1.00E-36		
Fe2O3(H)	4	159.692	1.00E-21		
BO2(-a)	6	42.809	4.68E-15		

Table B-4. (continued).

MgSO4*2H2O	4	156.393	5.05E-14		
MgO*Al2O3	4	142.266	1.00E-36		
MgO2	4	56.304	3.31E-23		
MgSO4*4H2O	4	192.423	2.59E-12		
MnO*Fe2O3	4	230.630	2.26E-25		
OH(-a)	6	17.008	2.92E-15		
Fe2MnO4	4	230.630	7.19E-26		
MnSO4*4H2O	4	223.056	2.49E-13		
MnO	4	70.937	5.49E-22		
MgO	4	40.304	2.23E-25		
MgO(M)	4	40.304	6.73E-26		
MnSO4*7H2O	4	277.102	4.15E-14		
FeSO4*H2O	4	169.920	1.91E-20		
Fe3O4	4	231.539	1.12E-29		
FeSO4	4	151.905	2.21E-23		
Fe2MgO4	4	199.997	1.97E-31		
H2SO4	4	98.073	1.02E-19		
CaO*2Al2O3	4	260.002	1.00E-36		
FeO	4	71.846	2.64E-27		
FeSO4*4H2O	4	223.965	3.38E-20		
Mn3O4	4	228.812	2.36E-28		
FeSO4*7H2O	4	278.011	1.28E-19		
OH(a)	6	17.007	9.99E-26		
CaO*Al2O3	4	158.041	1.00E-36		
CaO	4	56.079	3.77E-36		
CaCl2	3	110.986	3.64E-34		
Fe2(SO4)3	4	399.867	8.49E-35		
MnCl2*2H2O	3	161.874	4.02E-27		
MnCl2*4H2O	3	197.905	4.07E-26		
Al2(SO4)3	4	342.136	1.00E-36		
MgCl2*6H2O	3	203.302	1.05E-27		
CaCl2*6H2O	3	219.077	7.56E-27		
CaCl2*4H2O	3	183.047	4.24E-28		
MgCl2*4H2O	3	167.272	1.56E-30		
MgCl2*2H2O	3	131.241	8.50E-36		
MgCl2*H2O	3	113.226	1.00E-36		
FeCl2	3	126.753	1.00E-36		
*			*		
*			*		
*			*		
FeB	5	66.657	1.00E-36		
Fe2B	5	122.504	1.00E-36		
H2S(a)	6	34.076	1.00E-36		
PO4(-3a)	6	94.973	1.00E-36		
				gram precip per litre =	**31.11**

Table B-5. WM-189 TDS Drying @ 125ºC HSC OUTPUT

C:\My Documents\TAB HSC Folder\TAB HSC Calc\WM189liq2.OGI					
Date: 15 Aug 2002			**Data Set: 21**		
	Phase	**MW g/mol**	**Temperature: 125ºC**		
			(mol)	(g/l)	{out}
Ar(g)	1	39.948	3.26E+05		1.30E+07
H2O(g)	1	18.015	4.39E+01		7.91E+02
NO2(g)	1	46.006	3.94E+00		1.81E+02
HNO3(g)	1	63.013	3.05E-01		1.92E+01
NaNO3	4	84.995	1.96E-01	1.67E+01	
NaNO3(ia)	6	84.995	1.60E+00	1.36E+02	
O2(a)	6	31.999	9.79E-01		3.13E+01
Al(NO3)3(a)	6	212.996	3.06E-01	6.52E+01	
Na(+a)	6	22.989	2.88E-01	6.62E+00	
NO3(-a)	6	62.005	2.05E-01	1.27E+01	
KNO3	4	101.103	1.66E-01	1.68E+01	
Al2O3(C)	4	101.961	9.00E-02	9.18E+00	
Al2O3	4	101.961	7.93E-02	8.08E+00	
H(+a)	6	1.007	2.09E-05	2.11E-05	
K(+a)	6	39.098	5.43E-02	2.12E+00	
SO4(-2a)	6	96.059	8.04E-02	7.72E+00	
CaSO4	4	136.138	6.56E-02	8.93E+00	
HNO3(a)	6	63.013	3.40E-05	2.14E-03	
Al2O3(K)	4	101.961	7.72E-03	7.87E-01	
HBO2	4	43.817	7.71E-05	3.38E-03	
MnO2	4	86.937	2.00E-02	1.74E+00	
MgSO4(A)	4	120.363	1.68E-02	2.02E+00	
Al2O3(D)	4	101.961	5.44E-03	5.55E-01	
FeF(+2a)	6	74.844	4.19E-03	3.13E-01	
HF(g)	1	20.006	4.34E-03		8.68E-02
Fe2O3	4	159.692	5.78E-03	9.24E-01	
NaCl(a)	6	58.443	7.31E-05	4.27E-03	
FeCl2(+a)	6	126.752	1.01E-02	1.27E+00	
Al4B2O9	4	273.541	1.05E-02	2.86E+00	
MnSO4*H2O	4	169.011	7.68E-08	1.30E-05	
CaSO4(A)	4	136.138	6.62E-03	9.01E-01	
Cl2(g)	1	70.906	3.34E-04		2.37E-02
H2O	6	18.015	2.10E-04	3.78E-03	
MgSO4(B)	4	120.363	5.24E-03	6.31E-01	
Mn(+2a)	6	54.937	1.74E-07	9.57E-06	
H3BO2	4	45.833	1.77E-07	8.11E-06	
Al(+3a)	6	26.980	1.84E-03	4.96E-02	
MnSO4	4	150.996	1.81E-05	2.74E-03	
Cl(-a)	6	35.454	3.55E-05	1.26E-03	
CaSO4(B)	4	136.138	1.46E-03	1.99E-01	
AlF3	2	83.977	1.82E-03	1.53E-01	
HCl(g)	1	36.461	1.12E-04		4.10E-03
Al2O3(G)	4	101.961	3.66E-04	3.73E-02	
Al2(SO4)3	4	342.136	1.36E-03	4.64E-01	
Fe2(SO4)3	4	399.867	5.20E-04	2.08E-01	
CaSO4*0.5H2O(A)	4	145.145	1.26E-04	1.82E-02	
CaSO4*0.5H2O	4	145.145	1.12E-04	1.63E-02	
Al2O3*H2O	4	119.976	8.31E-04	9.96E-02	
Ar(a)	6	39.948	1.28E-04		5.09E-03
CaSO4*0.5H2O(B)	4	145.145	1.09E-04	1.58E-02	
NO(g)	1	30.006	9.94E-06		2.98E-04

Table B-5. (continued).

B2O3	4	69.618	6.87E-10	4.78E-08	
H3BO3	4	61.832	2.91E-10	1.80E-08	
N2O4(g)	1	92.011	1.02E-06		9.38E-05
N2(a)	6	28.013	1.23E-07		3.43E-06
CaSO4*2H2O	4	172.168	5.28E-11	9.09E-09	
F(-a)	6	18.999	4.23E-08	8.03E-07	
B2O3(A)	4	69.618	4.86E-11	3.38E-09	
AlO(+a)	6	42.980	1.05E-06	4.53E-05	
B2O3(G)	4	69.618	4.65E-11	3.23E-09	
Al18B4O33	4	1056.888	1.44E-08	1.52E-05	
H3BO3(a)	6	61.832	1.90E-10	1.18E-08	
H2SO4*3H2O	4	152.119	7.87E-20	1.20E-17	
HF(a)	6	20.006	4.58E-08	9.17E-07	
H2SO4	4	98.073	2.32E-12	2.27E-10	
Fe2O3*H2O	4	177.707	3.70E-08	6.57E-06	
Ca(+2a)	6	40.079	7.36E-09	2.95E-07	
MgSO4(a)	6	120.363	7.03E-09	8.46E-07	
Mn2O3	4	157.874	3.24E-11	5.11E-09	
BO2(-a)	6	42.809	1.63E-11	7.00E-10	
FeSO4	4	151.905	1.76E-09	2.67E-07	
H2SO4*4H2O	4	170.134	1.82E-23	3.09E-21	
MnO*Al2O3	4	172.899	2.14E-12	3.69E-10	
NaNO2	4	68.995	4.55E-12	3.14E-10	
MgSO4	4	120.363	1.96E-11	2.36E-09	
MnSO4*4H2O	4	223.056	2.11E-22	4.71E-20	
Ca(NO3)2	4	164.090	6.14E-11	1.01E-08	
Fe2O3(H)	4	159.692	7.74E-13	1.24E-10	
Mg(+2a)	6	24.304	2.35E-12	5.71E-11	
MgSO4*H2O	4	138.378	2.21E-12	3.06E-10	
FeSO4*H2O	4	169.920	6.13E-12	1.04E-09	
OH(-a)	6	17.008	1.42E-14	2.42E-13	
CaF2	2	78.077	1.19E-12	9.28E-11	
Fe(+2a)	6	55.846	1.30E-12	7.28E-11	
MnO*Fe2O3	4	230.630	1.63E-15	3.77E-13	
Fe2MnO4	4	230.630	7.04E-16	1.62E-13	
Mn(NO3)2	4	178.948	1.67E-15	2.99E-13	
HNO2(a)	6	47.013	2.35E-13	1.10E-11	
MnO	4	70.937	2.46E-16	1.74E-14	
Ca(NO3)2*2H2O	4	200.120	7.89E-19	1.58E-16	
Fe3O4	4	231.539	5.67E-17	1.31E-14	
Al2O3*3H2O	4	156.007	3.79E-14	5.91E-12	
MgCl(+a)	6	59.757	2.77E-15	1.65E-13	
Ca(NO3)2*3H2O	4	218.135	1.09E-22	2.38E-20	
FeO	4	71.846	1.72E-18	1.24E-16	
MgO*Al2O3	4	142.266	3.87E-21	5.51E-19	
MgSO4*2H2O	4	156.393	4.20E-18	6.58E-16	
MgO2	4	56.304	5.75E-21	3.24E-19	
Ca(NO3)2*4H2O	4	236.151	1.32E-26	3.12E-24	
CaO*2Al2O3	4	260.002	7.41E-24	1.93E-21	
Mn3O4	4	228.812	1.98E-21	4.54E-19	
MgO	4	40.304	2.03E-23	8.20E-22	
MgO(M)	4	40.304	8.62E-24	3.47E-22	
Fe2MgO4	4	199.997	1.46E-24	2.93E-22	
MnSO4*7H2O	4	277.102	1.00E-36	2.77E-34	
MgSO4*4H2O	4	192.423	4.45E-26	8.57E-24	
CaO*Al2O3	4	158.041	9.26E-27	1.46E-24	
Mg(NO3)2	4	148.315	5.07E-21	7.52E-19	
OH(a)	6	17.007	2.25E-22	3.83E-21	
FeSO4*4H2O	4	223.965	1.61E-25	3.61E-23	
Al(NO3)3*6H2O	4	321.087	1.13E-31	3.64E-29	
MgSO4*6H2O	4	228.454	3.39E-34	7.75E-32	

Table B-5. (continued).

CaO	4	56.079	3.14E-29	1.76E-27	
MgSO4*7H2O	4	246.469	1.00E-36	2.46E-34	
Mg(NO3)2*6H2O	4	256.406	1.00E-36	2.56E-34	
FeSO4*7H2O	4	278.011	1.00E-36	2.78E-34	
B3O3F3	2	137.423	3.99E-28	5.48E-26	
ClO3F(g)	1	102.450	3.92E-30		4.02E-28
CaSO3	4	120.138	8.51E-35	1.02E-32	
CaSO3*0.5H2O	4	129.146	1.70E-36	2.20E-34	
Fe3O4(H)	4	231.539	1.00E-36	2.32E-34	
MgSO3	4	104.363	1.00E-36	1.04E-34	
H2S(g)	1	34.076	1.00E-36		3.41E-35
CaCl2	3	110.986	1.00E-36	1.11E-34	
CaCl2*4H2O	3	183.047	1.00E-36	1.83E-34	
CaCl2*6H2O	3	219.077	1.00E-36	2.19E-34	
Ca(ClO3)2	3	206.982	1.00E-36	2.07E-34	
Ca(ClO4)2	3	238.981	1.00E-36	2.39E-34	
FeCl2	3	126.753	1.00E-36	1.27E-34	
FeCl3	3	162.206	1.00E-36	1.62E-34	
FeCl2*2H2O	3	162.783	1.00E-36	1.63E-34	
FeCl2*4H2O	3	198.814	1.00E-36	1.99E-34	
MgCl2*H2O	3	113.226	1.00E-36	1.13E-34	
MgCl2*2H2O	3	131.241	1.00E-36	1.31E-34	
MgCl2*4H2O	3	167.272	1.00E-36	1.67E-34	
MgCl2*6H2O	3	203.302	1.00E-36	2.03E-34	
MnCl2*2H2O	3	161.874	1.00E-36	1.62E-34	
MnCl2*4H2O	3	197.905	1.00E-36	1.98E-34	
*2CaO*Al2O3	4	214.120	1.00E-36	2.14E-34	
*3CaO*Al2O3	4	270.199	1.00E-36	2.70E-34	
*12CaO*7Al2O3	4	1386.682	1.00E-36	1.39E-33	
*3CaO*Al2O3*6H2(	4	378.291	1.00E-36	3.78E-34	
*4CaO*Al2O3*13H1	4	560.476	1.00E-36	5.60E-34	
*2CaO*Fe2O3	4	271.851	1.00E-36	2.72E-34	
CaSO3*2H2O	4	156.169	1.00E-36	1.56E-34	
MnSO4*5H2O	4	241.072	1.00E-36	2.41E-34	
FeB	5	66.657	1.00E-36	6.67E-35	
Fe2B	5	122.504	1.00E-36	1.23E-34	
H2S(a)	6	34.076	1.00E-36	3.41E-35	
NH4(+a)	6	18.038	1.00E-36	1.80E-35	
			TDS Estimate =	**302.9**	

Table B-6. Valences and molecular weights assumed in calculations.

Cations	MW	Valence
Acid	1.00794	1
Aluminum	26.98154	3
Antimony	121.757	3
Arsenic	74.92159	3
Barium	137.327	2
Beryllium	9.012182	2
Boron	10.811	3
Cadmium	112.411	2
Calcium	40.078	2
Cerium	140.115	3
Cesium	132.9054	1
Chromium	51.9961	3
Cobalt	58.9332	3
Copper	63.546	2
Gadolinium	157.25	3
Hafnium	178.49	4
Iron	55.847	3
Lead	207.2	2
Lithium	6.941	1
Magnesium	24.305	2
Manganese	54.93805	2
Mercury	200.59	2
Molybdenum	95.94	3
Nickel	58.6934	2
Niobium	92.90638	5
Palladium	106.42	2
Potassium	39.0983	1

Cations (cont'd)	MW	Valence
Ruthenium	101.07	3
Selenium	78.96	4
Silicon	28.0855	4
Silver	107.8682	1
Sodium	22.98977	1
Strontium	87.62	2
Tellurium	127.60	4
Thallium	204.3833	3
Thorium	232.038	4
Tin	118.71	2
Titanium	47.88	4
Uranium	237.44	6
Vanadium	50.9415	3
Zinc	65.39	2
Zirconium	91.224	4

ANIONS	MW	Valence
Chloride	35.4527	-1
Fluoride	18.9984	-1
Nitrate	62.00494	-1
Phosphorus	30.974	
Phosphate	94.97136	-3
Sulfur	32.06	
Sulfate	96.0636	-2
Oxygen	15.999	-2
Iodine	126.9045	-1